Presto 2.9 User’s Guide

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Abstract

Presto is a Lagrangian, three-dimensional explicit, transient dynamics code that is used to analyze solids subjected to large, suddenly applied loads. The code is designed for a parallel computing environment and for problems with large deformations, nonlinear material behavior, and contact. Presto also has a versatile element library that incorporates both continuum elements and structural elements. This user’s guide describes the input for Presto that gives users access to all the current functionality in the code. The environment in which Presto is built allows it to be coupled with other engineering analysis codes. Using a concept called scope, the input structure reflects the fact that Presto can be used in a coupled environment. The user’s guide describes how scope is implemented from the outermost to the innermost scopes. Within a given scope, the descriptions of input commands are grouped based on functionality of the code. For example, all material input command lines are described in a chapter of the user’s guide for all the material models that can be used in Presto.
Acknowledgments

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Chapter 1

Introduction

This document is a user’s guide for the code Presto. Presto is a three-dimensional transient dynamics code with a versatile element library, nonlinear material models, large deformation capabilities, and contact. It is built on the SIERRA Framework [1, 2]. SIERRA provides a data management framework in a parallel computing environment that allows the addition of capabilities in a modular fashion. Contact capabilities are parallel and scalable.

The Presto 2.9 User’s Guide provides information about the functionality in Presto and the command structure required to access this functionality in a user input file. This document is divided into chapters based primarily on functionality. For example, the command structure related to the use of various element types is grouped in one chapter; descriptions of material models are grouped in another chapter.

The input and usage of Presto is similar to that of the code Adagio [3]. Adagio is a three-dimensional quasi-static code with a versatile element library, nonlinear material models, large deformation capabilities, and contact. Adagio, like Presto, is built on the SIERRA Framework [1]. Contact capabilities for Adagio are also parallel and scalable. A significant feature of Adagio is that it offers a multilevel, nonlinear iterative solver.

Because of the similarities in input and usage between Presto and Adagio, the user’s guides for the two codes are structured in the same manner and share common material. (Once you have mastered the input structure for one code, it will be easy to master the syntax structure for the other code.) To maintain the commonality between the two user’s guides, we have used a variety of techniques. For example, references to Adagio may be found in the Presto user’s guide and vice versa, and the chapter order across the two guides is the same.

On the other hand, each of the two user’s guides is expressly tailored to the features of the specific code and documents the particular functionality for that code. For example, though both Presto and Adagio have contact functionality, the content of the chapter on contact in the two guides differs.

Important references for both Adagio and Presto are given in the references section at the end of this chapter. Adagio was preceded by the codes JAC and JAS3D; JAC is described in Reference 4; JAS3D is described in Reference 5. Presto was preceded by the code Pronto3D. Pronto3D is described in References 6 and 7. Some of the fundamental nonlinear technology used by both Presto and Adagio are described in References 8, 9, and 10. Currently, both Presto and Adagio
use the Exodus II database and the XDMF database; Exodus II is more commonly used than XDMF. (Other options may be added in the future.) The Exodus II database format is described in Reference 11, and the XDMF database format is described in Reference 12. Important information about contact is provided in the reference document for ACME [13]. ACME is a third-party library for contact.

One of the key concepts for the command structure in the input file is a concept referred to as scope. A detailed explanation of scope is provided in Section 1.2. Most of the command lines in Chapter 2 are related to a certain scope rather than to some particular functionality.

1.1 Document Overview

This document describes how to create an input file for Presto. Highlights of the document contents are as follows:

- Chapter 1 presents the overall structure of the input file, including conventions for the command descriptions, style guidelines for file preparation, and naming conventions for input files that reference the Exodus II database [11]. The chapter also gives an example of the general structure of an input file that employs the concept of scope.

- Chapter 2 explains some of the commands that are general to various applications based on the SIERRA Framework. These commands let you define scopes, functions, and coordinate systems, and they let you set up some of the main time control parameters (begin time, end time, time blocks) for your analysis. (Time control and time step control are discussed in more detail in Chapter 3.) Other capabilities documented in this chapter are available for calculating element distortion and for activating and deactivating functionality at different times throughout an analysis.

- Chapter 3 describes how to set the start time, end time, and time blocks for an analysis. This chapter also discusses various options for controlling the critical time step in Presto.

- Chapter 4 describes material models that can be used in conjunction with the elements in Presto and Adagio. Most of the material models have an interface that allows the models to be used by the elements in both codes. Even though a material model can be used by both codes, it may be that the use of the material model is better suited for one code rather than for the other code. For example, a material model set up to characterize behavior over a long time would be better suited for use in Adagio than in Presto. If a material model is better suited for one of the two codes, this information will be noted for the material model. In some cases, a material model may only be included in one of the two user’s guides. For example, there is a class of material models referred to as equation-of-state models. These models are designed for an explicit, transient dynamics code. The equation-of-state models are included in the Presto user’s guide but not in the Adagio user’s guide. Chapter 4 also discusses the application of temperature to a mesh, the computation of thermal strains (isotropic and anisotropic), and, for Presto, the deposition of energy for the equation-of-state material models.
1.1. DOCUMENT OVERVIEW

- Chapter 5 lists the elements in Presto and Adagio and describes how to set up commands to use the various options for the elements. Most elements can be used in either Presto or Adagio. If an element is available in one code but not the other, this information will be noted for the element. In some cases, an element may only be included in one of the two user’s guides. For example, Presto has a special element implementation referred to as smoothed particle hydrodynamics (SPH). The Presto user’s guide contains a section on SPH, but the Adagio user’s guide does not. Chapter 5 also includes descriptions of the commands for mass property calculations, element death, and mesh rebalancing. Two “element-like” capabilities are discussed in Chapter 5—torsional springs and rigid bodies. Although torsional springs and rigid bodies exhibit element-like behavior, they are really implemented as boundary conditions. From a user’s point of view, it is best to discuss the torsional-spring and rigid-body capabilities with elements.

- Chapter 6 documents how to use kinematic boundary conditions, force boundary conditions, initial conditions, and specialized boundary conditions.

- Chapter 7 discusses how to define interactions of contact surfaces.

- Chapter 8 details the various options for obtaining output.

- Chapter 9 provides an overview of the user subroutine functionality.

- Chapter 10 provides a sample input file from an analysis of 16 lead spheres being crushed together inside a steel box. This problem emphasizes large deformation and contact.

- Chapter 11 gives all the permissible Presto input lines in their proper scope.

- The index allows you to find information about command blocks and command lines. In general, single-level entries identify the page where the command syntax appears, with discussion following soon thereafter—on the same page or on a subsequent page. Page ranges are not provided in this index. Some entries consist of two or more levels. Such entries are typically based on context, including such information as the command blocks in which a command line appears, the location of the discussion related to a particular command line, and tips on usage. The PDF version of this document contains hyperlinked entries from the page numbers listed in the index to the text in the body of the document.

Note that all references cited within the text of Chapters 1 through 11 are listed at the end of the respective chapters rather than in a separate references chapter. The reference sections in the chapters are not necessarily edited so that they are specific to Adagio or Presto. Some chapters will have exactly the same set of references (even if not all are cited for a particular user’s guide), and some chapters will have the references tailored to the specific user’s guide.
1.2 Overall Input Structure

Presto is one of many mechanics codes built on the SIERRA Framework. The SIERRA Framework provides the capability to perform multiphysics analyses by coupling together SIERRA codes appropriate for the mechanics of interest. Input files may be set up for analyses using only Presto, or they may be set up to couple Presto and one or more other SIERRA analysis codes. For example, you might run Adagio to compute a stress state, and then use the results of this analysis as initial conditions for a Presto analysis. For a multiphysics analysis using Presto and Adagio, the time-step control, the mesh-related definitions, and the boundary conditions for both Presto and Adagio will all be in the same input file. Therefore, the input for Presto reflects the fact that it could be part of a multiphysics analysis. (Note that not all codes built on the SIERRA Framework can be coupled. Consult with the authors of this document to learn about the codes that can be coupled with Presto.)

To create files defining multiphysics analyses, the input files use a concept called “scope.” Scope is used to group similar commands; a scope can be nested inside another scope. The broadest scope in the input file is the domain scope. The domain scope contains information that can be shared among different physics. Examples of physics information that can be shared are definitions of functions and materials. Thus, in our above example of a coupled Presto/Adagio multiphysics analysis, both Adagio and Presto could reference functions to define such things as time histories for boundary conditions or stress-strain curves. Some of the functions could even be shared by these two applications. Both Presto and Adagio could also share information about materials.

Within the domain scope are two other important scopes: the procedure scope and the region scope. The region is nested inside the procedure, and the procedure is nested inside the domain. The procedure scope controls the overall analysis from the start time to the end time; the region scope controls a single time step. For a multiphysics analysis, the domain scope could contain several different procedures and several different regions.

Inside the procedure scope (but outside of the region scope) are commands that set the start time and the end time for the analysis.

Inside the region scope for Presto are such things as definitions for boundary conditions and contact. In a multiphysics analysis, there would be more than one region. In our Presto/Adagio example, there would be both a Presto region and an Adagio region, each within its respective procedures. The definitions for boundary conditions and contact and the mesh specification for Presto would appear in the Presto region; the definitions for boundary conditions and contact and the mesh specification for Adagio would appear in the Adagio region.

The input for Presto consists of command blocks and command lines. The command blocks define a scope. These command blocks group command lines or other command blocks that share a similar functionality. A command block will begin with an input line that has the word “begin”; the command block will end with an input line that has the word “end”. The domain scope, for example, is defined by a command block that begins with an input line of the following form:

\begin{verbatim}
BEGIN SIERRA my_problem
\end{verbatim}

The two character strings \texttt{BEGIN} and \texttt{SIERRA} are the key words for this command block. An input line defining a command block or a command line will have one or more key words. The string
my_problem is a user-specified name for this domain scope. The domain scope is terminated by an input line of the following form:

   END SIERRA my_problem

In the above input line, END and SIERRA are the key words to end this command block. The domain scope can also be terminated simply by using the following key word:

   END

The above abbreviated command line will be discussed in more detail in later chapters. There are similar input lines used to define the procedure and region scopes. Boundary conditions are another example where a scope is defined. A particular instance of a boundary condition for a prescribed displacement boundary condition is defined with a command block. The command block for the boundary condition begins with an input line of the form:

   BEGIN PRESCRIBED DISPLACEMENT

and ends with an input line of either of the following forms:

   END PRESCRIBED DISPLACEMENT
   END

Command lines appear within the command blocks. The command lines typically have the form keyword = value, where value can be a real, an integer, or a string. In the previous example of the prescribed displacement boundary condition, there would be command lines inside the command block that are used to set various values. For example, the boundary condition might apply to all nodes in node set 10, in which case there would be a command line of the following form:

   NODE SET = nodelist_10

If the prescribed displacement were to be applied along a given component direction, there would be a command line of this form:

   COMPONENT = X

The form above would specify that the prescribed displacement would be in the $x$-direction. Finally, if the displacement magnitude is described by a time history function with the name cosine_curve, there would be a command line of this form:

   FUNCTION = cosine_curve

The command block for the boundary condition with the appropriate command lines would appear as follows:

   BEGIN PRESCRIBED DISPLACEMENT
      NODE SET = nodelist_10
      COMPONENT = X
      FUNCTION = cosine_curve
   END PRESCRIBED DISPLACEMENT

It is possible to have a command line with the same key words appearing in different scopes. For example, we might have a command line identified by the word TYPE in two or more different
scopes. The command line would perform different functions based on the scope in which it appeared, and the associated value could be different in the two locations.

The input lines are read by a parser that searches for recognizable key words. If the key words in an input line are not in the list of key words used by Presto to describe command blocks and command lines, the parser will generate an error. A set of key words defining a command line or command block for Presto that is not in the correct scope will also cause a parser error. For example, the key words `STEP INTERVAL` define a valid command line in the scope of the `TIME CONTROL` command block. However, if this command line was to appear in the scope of one of the boundary conditions, it would not be in the proper scope, and the parser would generate an error. Once the parser has an input line with any recognizable key words in the proper scope, a method can be called that will handle the input line.

There is an initial parsing phase that checks only the parser syntax. If the parser encounters a command line it cannot parse within a certain scope, the parser will indicate it cannot recognize the command line and will list the various command lines that can appear within that scope. The initial parsing phase will catch errors such as the one described in the previous paragraph (a command line in the wrong scope). It will also catch misspelled key words. The initial parsing does not catch some other types of errors, however. If you have specified a value on a command line that is out of a specified range for that command line, the initial parsing will not catch this error. If you have some combination of command lines within a command block that is not allowed, the initial parsing will not catch this error. These other errors are caught after the initial parsing phase and are handled one error at a time.
1.3 Conventions for Command Descriptions

The conventions below are used to describe the input commands for Presto. A number of the individual command lines discussed in the text appear on several text lines. In the text of this document, the continuation symbols that are used to continue lines in an actual input file (\# and \\$, Section 1.4.2) are not used for those instances where the description of the command line appears on several text lines. The description of command lines will clearly indicate all the key words, delimiters, and values that constitute a complete command line. As an example, the DEFINE POINT command line (Section 2.1.6) is presented in the text as follows:

```
DEFINE POINT <string>point_name WITH COORDINATES
<real>value_1 <real>value_2 <real>value_3
```

If the DEFINE POINT command line were used as a command line in an input file and spread over two input lines, it would appear, with actual values, as follows:

```
DEFINE POINT center WITH COORDINATES \\#
10.0 144.0 296.0
```

In the above example, the \\# symbol implies the first line is continued onto the second line.

1.3.1 Key Words

The key word or key words for a command are shown in uppercase letters. For actual input, you can use all uppercase letters for the key words, all lowercase letters for the key words, or some combination of uppercase and lowercase letters for the key words.

1.3.2 User-Specified Input

The input that you supply is typically shown in lowercase letters. (Occasionally, uppercase letters may be used for user input for purposes of clarity or in examples.) The user-supplied input may be a real number, an integer, a string, or a string list. For the command descriptions, a type appears before the user input. The type (real, integer, string, string list) description is enclosed by angle brackets, <>, and precedes the user-supplied input. For example:

```
<real>value
```

indicates that the quantity value is a real number. For the description of an input command, you would see the following:

```
FUNCTION = <string>function_name
```

Your input would be

```
FUNCTION = my_name
```

if you have specified a function name called my_name.

Valid user input consists of the following:
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<integer> Integer data is a single integer number.

<real> Real data is a single real number. It may be formatted with the usual conventions, such as 1234.56 or 1.23456e+03.

<string> String data is a single string.

<string list> A string list consists of multiple strings separated by white space, a comma, a tab, or white space combined with a comma or a tab.

1.3.3 Optional Input

Anything in an input line that is enclosed by square brackets, [ ], represents optional input within the line. Note, however, that this convention is not used to identify optional input lines. Any command line that is optional (in its entirety) will be described as such within the text.

1.3.4 Default Values

A value enclosed by parentheses, (), appearing after the user input denotes the default value. For example:

\[ \text{SCALE FACTOR} = <\text{real}>scale\_factor(1.0) \]

implies the default value for \text{scale\_factor} is 1.0. Any value you specify will overwrite the default.

For your actual input file, you may simply omit a command line if you want to use the default value associated with the command line. For example, there is a \text{TIME STEP SCALE FACTOR} command line used to set one of the time control parameters; the parameter for this command line has a default value of 1.0. If you want to use the default value of 1.0 for this parameter, you do not have to include the \text{TIME STEP SCALE FACTOR} command line in the \text{TIME CONTROL} command block.

1.3.5 Multiple Options for Values

Quantities separated by the | symbol indicate that one and only one of the possible choices must be selected. For example:

\[ \text{EXPANSION RADIUS} = <\text{string}>\text{SPHERICAL}|\text{CYLINDRICAL} \]

implies that expansion radius must be defined as \text{SPHERICAL} or \text{CYLINDRICAL}. One of the values must appear. This convention also applies to some of the command options within a begin/end block. For example:
1.3. CONVENTIONS FOR COMMAND DESCRIPTIONS

\[
\text{SURFACE} = \text{<string>surface_name|} \\
\text{NODE SET} = \text{<string>nodelist_name}
\]

in a command block specifies that either a surface or a node set must be specified.

Quantities separated by the / symbol can appear in any combination, but any one quantity in the sequence can appear only once. For example,

\[
\text{COMPONENTS} = \text{<string>X/Y/Z}
\]

implies that components can equal any combination of X, Y, and Z. Any value (X or Y or Z) can appear at most once, and at least one value of X, Y, or Z must appear. Some examples of valid expressions in this case are as follows:

\[
\begin{align*}
\text{COMPONENTS} &= \text{Z} \\
\text{COMPONENTS} &= \text{Z X} \\
\text{COMPONENTS} &= \text{Y X Z} \\
\text{COMPONENTS} &= \text{Z Y X}
\end{align*}
\]

An example of an invalid expression would be the following:

\[
\text{COMPONENTS} = \text{Y Y Z}
\]

1.3.6 Set of Command Lines

In some of the command blocks, it may be possible to select from a set of command lines to activate some functionality within the command block. In the boundary conditions, a boundary condition may be applied to a group of nodes. This group of nodes can be defined by some collection of command lines that are Boolean operations to add or delete nodes to the group. The command lines that are the Boolean operations to define the group of nodes are described in detail in the introduction to the chapter on boundary conditions, e.g., in Section 6.1.1. In the description of the command blocks for the boundary conditions, we denote this set of command lines by enclosing a name for the set of command lines in curly braces, \{\}. Therefore, the description of a command block for a kinematic boundary condition may have a line of the form:

\[
\{\text{node set commands}\}
\]

to indicate that the user can insert some arbitrary combination of command lines from the set of command lines defined as node set commands.

We will use \{\} to enclose some named set of command lines or some description of a set of command lines.

1.3.7 Known Issues and Warnings

Where there are known issues with the code, these are documented in the following manner:
**Known Issue:** A description of the known issue with the code would be provided here.

Similarly, warnings regarding usage of code features that are not defective, but must be used with care because of their nature, are documented as follows:

**Warning:** A description of the warning related to the usage of a code feature would be provided here.
1.4 Style Guidelines

This section gives information that will affect the overall organization and appearance of your input file. It also contains recommendations that will help you construct input files that are readable and easy to proof.

1.4.1 Comments

A comment is anything between the # symbol or the $ symbol and the end-of-line. If the first nonblank character in a line is a # or $, the entire line is a comment line. You can also place a # or $ (preceded by a blank space) after the last character in an input line used to define a command block or command line.

1.4.2 Continuation Lines

An input line can be continued by placing a \# pair of characters (or \$) at the end of the line. The following line is then taken to be a continuation of the preceding line that was terminated by the \# or \$. Note that everything after the line-continuation pair of characters is discarded, including the end-of-line.

1.4.3 Case

Almost all the character strings in the input lines are case insensitive. For example, the BEGIN SIERRA key words could appear as one of the following:

```
BEGIN SIERRA
begin sierra
Begin Sierra
```

You could specify a SIERRA command block with:

```
BEGIN SIERRA BEAM
```

and terminate the command block with this input line:

```
END SIERRA beam
```

Case is important only for file name specifications. If you have defined a restart file with uppercase and lowercase letters and want to use this file for a restart, the file name you use to request this restart file must exactly match the original definition you chose.

1.4.4 Commas and Tabs

Commas and tabs in input lines are ignored.
1.4.5 Blank Spaces

We highly recommend that everything be separated by blank spaces. For example, a command line of the form

```
node set = nodelist_10
```

is recommended over the following forms:

```
node set= nodelist_10
node set = nodelist_10
```

Both of the above two lines are correct, but it is easier to check the first form (the equal sign surrounded by blank space) in a large input file.

The parser will accept the following line:

```
BEGIN SIERRABEAM
```

However, it is harder to check this line for the correct spelling of the key words and the intended domain name than this line:

```
BEGIN SIERRA BEAM
```

It is possible to introduce hard-to-detect errors because of the way in which the blank spaces are handled by the command parser. Suppose you type

```
begin definition for functions my_func
```

rather than the following correct form:

```
begin definition for function my_func
```

For the incorrect form of this command line (in which `functions` is used rather than `function`), the parser will generate a string name of

```
s my_func
```

for the function name rather than the following expected name:

```
my_func
```

If you attempt to use a function named `my_func`, the parser will generate an error because the list of function names will include `s my_func` but not `my_func`.

1.4.6 General Format of the Command Lines

In general, command lines have the following form:

```
keyword = value
```

This pattern is not always followed, but it describes the vast majority of the command lines.
1.4.7 Delimiters

The delimiter used throughout this document is “=” (the equal sign). Typically, but not always, the = separates key words from input values in a command line. Consider the following command line:

```
COMPONENTS = X
```

Here, the key word COMPONENTS is separated from its value, a string in this case, by the =. Some command lines do allow for other delimiters. The use of these alternate delimiters is not consistent, however, throughout the various command lines. (This lack of consistency has the potential for introducing errors in this document as well as in your input.) The = provides a strong visual cue for separating key words from values. By using the = as a delimiter, it is much easier to proof your input file. It also makes it easier to do “cut and paste” operations. If you accidentally delete =, it is much easier to detect than accidentally removing part of one of the other delimiters that could be used.

1.4.8 Order of Commands

There are no requirements for ordering the commands. Both the input sequence:

```
BEGIN PRESCRIBED DISPLACEMENT
  NODE SET = nodelist_10
  COMPONENT = X
  FUNCTION = cosine_curve
END PRESCRIBED DISPLACEMENT
```

and the input sequence:

```
BEGIN PRESCRIBED DISPLACEMENT
  FUNCTION = cosine_curve
  COMPONENT = X
  NODE SET = nodelist_10
END PRESCRIBED DISPLACEMENT
```

are valid, and they produce the same result. Remember, that command lines and command blocks must appear in the proper scope.

1.4.9 Abbreviated END Specifications

It is possible to terminate a command block without including the key word or key words that identify the block. You could define a specific instance of the prescribed displacement boundary condition with:

```
BEGIN PRESCRIBED DISPLACEMENT
```
and terminate it simply with:

END

as opposed to the following specification:

END PRESCRIBED DISPLACEMENT

Both the short termination (END only) and the long termination (END followed by identification, or name, of the command block) are valid. It is recommended that the long termination be used for any command block that becomes large. The RESULTS OUTPUT command block described in later chapters can become fairly lengthy, so this is probably a good place to use the long termination. For most boundary conditions, the command block will typically consist of five lines. In such cases, the short termination can be used. Using the long termination for the larger command blocks will make it easier to proof your input files. If you use the long termination, the text following the END key word must exactly match the text following the BEGIN key word. You could not have BEGIN PRESCRIBED DISPLACEMENT paired with an END PRESCRIBED DISPL to define the beginning and ending of a command block.

1.4.10 Indentation

When constructing an input file, it is useful, but not required, to indent a scope that is nested inside another scope. Command lines within a command block should also be indented in relation to the lines defining the command block. This will make it easier to construct the input file with everything in the correct scope and with all the command blocks in the correct structure.
1.5 Naming Conventions Associated with the Exodus II Database

When the mesh file has an Exodus II format, there are three basic conventions that apply to user input for various command lines. First, for a mesh file with the Exodus II format, the Exodus II side set is referenced as a surface. In SIERRA, a surface consists of element faces plus all the nodes and edges associated with these faces. A surface definition can be used not only to select a group of faces but also to select a group of edges or a group of nodes that are associated with those faces. In the case of boundary conditions, a surface definition can be used not only to apply boundary conditions that typically use surface specifications (pressure) but also to apply boundary conditions for what are referred to as nodal boundary conditions (fixed displacement components). For nodal boundary conditions that use the surface specification, all the nodes associated with the faces on a specific surface will have this boundary condition applied to them. The specification for a surface identifier in the following chapters is surface_name. It typically has the form surface_integerid, where integerid is the integer identifier for the surface. If the side set identifier is 125, the value of surface_name would be surface_125. It is also possible to generate an alias for the side set and use this for surface_name. If surface_125 is aliased to outer_skin, then surface_name becomes outer_skin in the actual input line. It is also possible to name a surface in some mesh generation programs and that name can be used in the input file.

Second, for a mesh file with the Exodus II format, the Exodus II node set is still referenced as a node set. A node set can be used only for cases where a group of nodes needs to be defined. The specification for a node set identifier in the following chapters is nodelist_name. It typically has the form nodelist_integerid, where integerid is the integer identifier for the node set. If the node set number is 225, the value of nodelist_name would be nodelist_225. It is also possible to generate an alias for the node set and use this for nodelist_name. If nodelist_225 is aliased to inner_skin, then nodelist_name becomes inner_skin in the actual input line. It is also possible to name a nodelist in some mesh generation programs and that name can be used in the input file.

Third, an element block is referenced as a block. The specification for an element block identifier in the following chapters is block_name. It typically has the form block_integerid, where integerid is the integer identifier for the block. If the element block number is 300, the value of block_name would be block_300. It is also possible to generate an alias for the block and use this for block_name. If block_300 is aliased to big_chunk, then block_name becomes big_chunk in the actual input line. It is also possible to name an element block in some mesh generation programs and that name can be used in the input file.

A group of elements can also be used to select other mesh entities. In SIERRA, a block consists of elements plus all the faces, edges, and nodes associated with the elements. The block and surface concepts are similar in that both have associated derived quantities. Chapters 6 and 7 show how this concept of derived quantities is used in the input command structure.

---

1See the ALIAS command in Section 5.1.1.1
1.6 Major Scope Definitions for an Input File

The typical input file will have the structure shown below. The major scopes—domain, procedure, and region—are delineated with input lines for command blocks. Comment lines are included that indicate some of the key scopes that will appear within the major scopes. Note the indentation used for this example.

```
BEGIN SIERRA <string>some_name
  #
  # All command blocks and command lines in the domain
  # scope appear here. The PROCEDURE PRESTO command
  # block is the beginning of the next scope.
  #
  # function definitions
  # material descriptions
  # description of mesh file
  #
BEGIN PROCEDURE PRESTO <string>procedure_name
  #
  # time step control
  #
BEGIN REGION PRESTO <string>region_name
  #
  # All command blocks and command lines in the
  # region scope appear here
  #
  # specification for output of result
  # specification for restart
  # boundary conditions
  # definition of contact
  #
END [REGION PRESTO <string>region_name]
END [PROCEDURE PRESTO <string>procedure_name]
END [SIERRA <string>some_name]
```
1.7 Input/Output Files

The primary user input to Presto is the input file introduced in this chapter. Throughout this document, we explain how to construct a valid input file. It is important to be aware that Presto also processes a number of other types of input files and produces a variety of output files. These additional files are also discussed in this document where applicable. Figure 1.1 presents a simple schematic diagram of the various input and output files in Presto. Both Adagio and Presto use the same file structure. Therefore, in Figure 1.1, we indicate that the code (graphically represented by the central cylinder) can be either Presto or Adagio.

As shown in Figure 1.1, Presto uses the input file, mesh files, restart files, and user subroutine files. The input file, which is required, is a set of valid Presto command lines. Another required input is a mesh file, which provides a description of the finite element mesh for the object being analyzed. Restart and user subroutine files are optional inputs. The restart functionality lets you break an analysis from the start time to the termination time into a sequence of runs. The files generated by the restart functionality contain a complete state description for a problem at various analysis times, which we will refer to as restart times. You can restart Presto at any of these restart times because the complete state description is known (see Chapter 8). The user subroutine files let you build and incorporate specialized functionality into Presto (Chapter 9).

As also shown in Figure 1.1, Presto can generate a number of files. These include results files, history files, restart files, a log file, and an output file. Typically, only the log file and the output file are produced automatically. Generation of the other types of files is based on user settings in the input file for the particular kinds of output desired. Results files provide the values of global variables, element variables, and node variables at specified times (see Chapter 8). History files will also provide values of global variables, element variables, and node variables at specified times (see Chapter 8). History files are set up to provide a specific value at a specific node, for example, whereas results files provide a nodal value for large subsets of nodes or, more typically, all nodes. History files provide a much more limited set of information than results files. As noted above, restart files can be generated at various analysis times. The log file contains a variety of information...
such as the Presto version number, a listing of the input file, initialization information, some model information (mass, critical time steps for element blocks, etc.), and information at various time steps. At every $n$th step, where $n$ is user selected, the log file gives the current analysis time; the current time step; the kinetic, internal, and external energies; the error in the energy; and computing time information. You can monitor step information in the log file to gain information about how your analysis is progressing. The output file contains error information.
1.8 Obtaining Support

Support for all SIERRA Mechanics codes, including Presto, can be obtained by contacting the SIERRA Mechanics user support hotline by email at sierra-help@sandia.gov, or by telephone at (505)845-1234.
1.9 References


Chapter 2

General Commands

The commands described in this section appear in the domain or procedure scope or control some general functionality in Presto.

2.1 Domain Scope

These commands are used to set up some of the fundamentals of the Presto input. The commands are physics independent, or at least can be shared between physics. The commands lie in the domain scope, not in the procedure or region scope.

2.1.1 SIERRA Command Block

```
BEGIN SIERRA <string>name
#
# All other command blocks and command lines
# appear within the domain scope defined by
# begin/end sierra.
#
END [SIERRA <string>name]
```

All input commands must occur within a SIERRA command block. The syntax for beginning the command block is:

```
BEGIN SIERRA <string>name
```

and for terminating the command block is as follows:

```
END [SIERRA <string>name]
```

In these input lines, name is a name for the SIERRA command block. All other commands for the analysis must be within this command block structure. The name for the SIERRA command block is often a descriptive name that identifies the analysis. The name is not currently used anywhere else in the file and is completely arbitrary.
2.1.2 Title

TITLE <string list>title

To permit a fuller description of the analysis, the input has a TITLE command line for the analysis, where title is a text description of the analysis. The title is transferred to the results file.

2.1.3 Restart Control

The restart capability in Presto allows a user to run an analysis up to a certain time, stop the analysis at this time, and then restart the analysis from this time. Restart can be used to break a long-running analysis into several smaller runs so that the user can examine intermediate results before proceeding with the next step. Restart can also be used in case of abnormal termination. If a restart file has been written at various intervals throughout the analysis up to the point where the abnormal termination has occurred, you can pick a restart time before the abnormal termination and restart the problem from there. Thus, users do not have to go back to the beginning of the analysis, but can continue the analysis at some time well into the analysis. With the restart capability, you will generate a sequence of restart runs. Each run can have its own set of restart, results, and history files.

When using the restart capability, you can reset a number of the parameters in the input file. However, not all parameters can be reset. Users should exercise care in resetting parameters in the input file for a restart. You will want to change parameters if you have encountered an abnormal termination. You may want to change certain parameters, hourglass control for example, to see whether you can prevent the abnormal termination and continue the analysis past the abnormal termination time you had previously encountered.

The use of the restart capability involves commands in both the domain scope and the region scope. One of two restart command lines, RESTART or RESTART TIME, appears in the domain scope. A command block in the region scope, the RESTART DATA command block, specifies restart file names and the frequency at which the restart files will be written. The RESTART DATA command block is described in Section 8.4. This section gives a brief discussion of the command lines that appear in the domain scope. For a full discussion of all the command lines used for restart, consult with Chapter 8. The use of some of the command lines in the RESTART DATA command block depends on the command line, either RESTART or RESTART TIME, you select in the domain scope.

If you specify a time from a specific restart file for the restart, you will use the RESTART TIME command line described in Section 2.1.3.1. If you select the automatic restart option, you will use the RESTART command line described in Section 2.1.3.2. The command lines for both of these methods are in the domain scope. All other commands for restart are in the region scope in the RESTART DATA command block.

For restarts specified with a restart time from a specific restart file, you will have to be concerned about overwriting information in existing files. The issue of overwriting information is discussed in Chapter 8. In general, you will want to have a restart file (or files in the case of parallel runs)
for each run in a sequence of runs you create with the restart option. You will want to preserve all restart files you have written prior to any given run in a sequence of restart runs. The easiest way to preserve prior restart information is with the use of the \texttt{RESTART} command line. How you preserve previous restart information is discussed in detail in Chapter 8.

The amount of data written at a restart time is quite large. The restart data written at a given time is a complete description of the state for the problem at that time. The restart data includes not only information such as displacement, velocity, and acceleration, but also information such as element stresses and all the state variables for the material model associated with each element.

### 2.1.3.1 Restart Time

\texttt{RESTART TIME = <real>restart\_time}

The \texttt{RESTART TIME} command line is used to specify a time from a specific restart file for the restart run. This restart option will pick the restart time on the restart file that is closest to the user-specified time on the \texttt{RESTART TIME} command line. If the user specifies a restart time greater than the last time written to a restart file, then the last time written to the restart file is picked as the restart time. Use of this command line can result in previous restart information being overwritten. To prevent the overwriting of existing restart files, you can specify both an input restart file and an output restart file (and rename the results and history files) for the various restarts. The use of the \texttt{RESTART TIME} command line requires the user to be more active in the management of the file names to prevent the overwriting of restart, results, and history files. The automatic restart feature (e.g., the \texttt{RESTART} command line in Section 2.1.3.2) prevents the overwriting of restart, results, and history files. Consult with Section 8.4 for a full discussion of implementing the restart capability.

### 2.1.3.2 Automatic Restart

\texttt{RESTART = AUTOMATIC}

The \texttt{RESTART} command line automatically selects for restart the last restart time written to the last restart file. The automatic restart feature lets the user restart runs with minimal changes to the input file. The only quantity that must be changed to move from one restart to another is the termination time. The \texttt{RESTART} command line manages the restart files so as not to write over any previous restart files. It also manages the results and history files so as not to write over any previous results or history files. Consult with Section 8.4 for a full discussion of implementing the restart capability.

### 2.1.4 User Subroutine Identification

\texttt{USER SUBROUTINE FILE = <string>file\_name}
This command line is a part of a set of commands that are used to implement the user subroutine functionality. The string `file_name` identifies the name of the file that contains the FORTRAN code of one or more user subroutines.

To understand how this command line is used, see Chapter 9.

### 2.1.5 Functions

```
BEGIN DEFINITION FOR FUNCTION <string>function_name
  TYPE = <string>CONSTANT|PIECEWISE LINEAR|
    PIECEWISE CONSTANT|ANALYTIC
  ABSCISSA = <string>abscissa_label
  ORDINATE = <string>ordinate_label
  BEGIN VALUES
    <real>value_1  [<real>value_2
    <real>value_3  <real>value_4
    ...              <real>value_n]
  END [VALUES]
  AT DISCONTINUITY EVALUATE TO <string>LEFT|RIGHT
  EVALUATE EXPRESSION = <string>analytic_expression1; analytic_expression2;...;
  END [DEFINITION FOR FUNCTION <string>function_name]
```

A number of Presto features are driven by a user-defined description of the dependence of one variable on another. For instance, the prescribed displacement boundary condition requires the definition of a time-versus-displacement relation, and the thermal strain computations require the definition of a thermal-strain-versus-temperature relation. SIERRA provides a general method of defining these relations as functions using the `DEFINITION FOR FUNCTION` command block, as shown above.

There is no limit to the number of functions that can be defined. All function definitions must appear within the domain scope.

A description of the various parts of the `DEFINITION FOR FUNCTION` command block follows:

- The string `function_name` is a user-selected name for the function that is unique to the function definitions within the input file. This name is used to refer to this function in other locations in the input file.

- The `TYPE` command line has four options to define the type of function. The value of this string can be `CONSTANT`, `PIECEWISE LINEAR`, `PIECEWISE CONSTANT`, or `ANALYTIC`.

- The `ABSCISSA` command line provides a descriptive label for the independent variable (x-axis) with the string `abscissa_label`. This command line is optional.

- The `ORDINATE` command line provides a descriptive label for the dependent variable (y-axis) with the string `ordinate_label`. This command line is optional.
2.1. DOMAIN SCOPE

- The VALUES command block consists of the real values value_1 through value_n, which describe the function. This command block must be used if the value on the TYPE command line is CONSTANT, PIECEWISE LINEAR, or PIECEWISE CONSTANT. For a CONSTANT function, only one value is needed. For a PIECEWISE LINEAR or PIECEWISE CONSTANT function, the values are (x, y) pairs of data that describe the function. The values are nested inside the VALUES command block.

![Figure 2.1: Piecewise linear and piecewise constant functions](image)

A PIECEWISE LINEAR function performs linear interpolations between the provided value pairs; a PIECEWISE CONSTANT function is constant valued between provided value pairs. Figure 2.1 (a) shows an example of a piecewise linear function, and Figure 2.1 (b) shows an example of a piecewise constant function.

In the case of a PIECEWISE LINEAR or PIECEWISE CONSTANT function, for any abscissa value passed to the function that is greater than the last abscissa value in the VALUES command block, the last ordinate value is used for the function value. For example, suppose a piecewise linear function named my_func describes a time history for a pressure load where the pressure increases from 0 to 50,000 psi from time 0.0 sec to time 1.0 × 10⁻³ sec. The last time specified in the function is 1.0 × 10⁻³. Now, suppose our final analysis time is 2.0 × 10⁻³ sec. Then, from the time 1.0 × 10⁻³ to the time 2.0 × 10⁻³, the value for this function (my_func) will be 50,000 psi.

- For a piecewise constant function, a constant value segment ends on the left hand side of an abscissa value and a new constant value segment begins on the right hand side of the same abscissa value. (This transition from one constant value to another is indicated by the dotted line in Figure 2.1 (b).) When an abscissa falls at a point where there are two ordinate values, the function returns, by default, the ordinate of the value pair that has the lower-valued abscissa. The AT DISCONTINUITY EVALUATE TO overrides this default behavior at an abscissa with two ordinate values. The command line can have a value of either LEFT or RIGHT. If LEFT is specified, the ordinate value to the left of the abscissa is used; if RIGHT is specified, the ordinate value to the right of the abscissa is used.

- The EVALUATE EXPRESSION command line consists of one or more user-supplied algebraic
expressions. This command line must be used if the value on the TYPE command line is ANALYTIC. See the rules and options for composing algebraic expressions discussed below.

Importantly, a DEFINITION FOR FUNCTION command block cannot contain both a VALUES command block and an EVALUATE EXPRESSION command line.

**Rules and options for composing algebraic expressions.** If you choose to use the EVALUATE EXPRESSION command line, you will need to write the algebraic expressions. The algebraic expressions are written using a C-like format. Each algebraic expression is terminated by a semi-colon(;). The entire set of algebraic expressions, whether a single expression or several, is enclosed in a single set of double quotes(" ").

An expression is evaluated with x as the independent variable. We first provide several simple examples and then list the options available in the algebraic expressions.

Example: Return sin(x) as the value of the function.

```
begin definition for function fred
  type is analytic
  evaluate expression is ``sin(x);''
end definition for function fred
```

In this example, the commented out table is equivalent to the evaluated expression:

```
begin definition for function pressure
  type is analytic
  evaluate expression is ``x <= 0.0 ? 0.0 : (x < 0.5 ? x*200.0 : 100.0);''
  # begin values
  # 0.0 0.0
  # 0.5 100.0
  # 1.0 100.0
  # end values
end definition for function pressure
```

The following functionality is currently implemented for the expressions:

**Operators**

```
+ - * / == != > < >= <= ! & | && || ? :
```

**Parentheses**

```
()
```

**Math functions**
2.1. **DOMAIN SCOPE**

- `abs(x)`, absolute value of `x`
- `mod(x, y)`, modulus of `x`\|`y`
- `ipart(x)`, integer part of `x`
- `fpart(x)`, fractional part of `x`

**Power functions**

- `pow(x, y)`, `x` to the `y` power
- `pow10(x)`, `x` to the `10` power
- `sqrt(x)`, square root of `x`

**Trigonometric functions**

- `acos(x)`, arccosine of `x`
- `asin(x)`, arcsine of `x`
- `atan(x)`, arctangent of `x`
- `atan2(y, x)`, arctangent of `y`\|`x`, signs of `x` and `y` determine quadrant (see `atan2` man page)
- `cos(x)`, cosine of `x`
- `cosh(x)`, hyperbolic cosine of `x`
- `sin(x)`, sine of `x`
- `sinh(x)`, hyperbolic sine of `x`
- `tan(x)`, tangent of `x`
- `tanh(x)`, hyperbolic tangent of `x`

**Logarithm functions**

- `log(x)`, natural logarithm of `x`
- `ln(x)`, natural logarithm of `x`
- `log10(x)`, the base `10` logarithm of `x`
- `exp(x)`, `e` to the `x` power

**Rounding functions**

- `ceil(x)`, smallest integral value not less than `x`
- `floor(x)`, largest integral value not greater than `x`

**Random functions**

- `rand()`, random number between `0.0` and `1.0`, not including `1.0`
- `randomize()`, random number between `0.0` and `1.0`, not including `1.0`
- `srand(x)`, seeds the random number generator

**Conversion functions**
deg(x), converts radians to degrees
rad(x), converts degrees to radians
recttopolr(x, y), magnitude of vector x, y
recttopola(x, y), angle of vector x, y
poltorectx(r, theta), x coordinate of angle theta at
distance r
poltorecty(r, theta), y coordinate of angle theta at
distance r

Constants. There are two predefined constants that may be used in an expression. These two
constants are $e$ and $\pi$.

\[
e = e = 2.7182818284...
\]
\[
\pi = \pi = 3.1415926535...
\]

2.1.6 Axes, Directions, and Points

\begin{verbatim}
DEFINE POINT <string>point_name WITH COORDINATES
   <real>value_1  <real>value_2  <real>value_3
DEFINE DIRECTION <string>direction_name WITH VECTOR
   <real>value_1  <real>value_2  <real>value_3
DEFINE AXIS <string>axis_name WITH POINT
   <string>point_1  POINT  <string>point_2
DEFINE AXIS <string>axis_name WITH POINT
   <string>point  DIRECTION  <string>direction
\end{verbatim}

A number of Presto features require the definition of geometric entities. For instance, the pre-
scribed displacement boundary condition requires a direction definition, and the cylindrical veloc-
ity initial condition requires an axis definition. Currently, Presto input permits the definition of
points, directions, and axes. Definition of these geometric entities occurs in the domain scope.

The DEFINE POINT command line is used to define a point:

\begin{verbatim}
DEFINE POINT <string>point_name WITH COORDINATES
   <real>value_1  <real>value_2  <real>value_3
\end{verbatim}

where

- The string point_name is a name for this point. This name must be unique to all other
  points defined in the input file.
- The real values value_1, value_2, and value_3 are the $x$, $y$, and $z$ coordinates of the
  point.

The DEFINE DIRECTION command line is used to define a direction:
2.1. DOMAIN SCOPE

DEFINE DIRECTION <string>direction_name WITH VECTOR
   <real>value_1 <real>value_2 <real>value_3

*where*

- The string `direction_name` is a name for this direction. This name must be unique to all other directions defined in the input file.

- The real values `value_1`, `value_2`, and `value_3` are the $x$, $y$, and $z$ magnitudes of the direction vector.

There are two command lines that can be used to define an axis. The first `DEFINE AXIS` command line uses two points:

```
DEFINE AXIS <string>axis_name WITH POINT
   <string>point_1 POINT <string>point_2
```

*where*

- The string `axis_name` is a name for this axis. This name must be unique to all other axes defined in the input file.

- The strings `point_1` and `point_2` are the names for two points defined in the input file via a `DEFINE POINT` command line.

The second `DEFINE AXIS` command line uses a point and a direction:

```
DEFINE AXIS <string>axis_name WITH POINT
   <string>point DIRECTION <string>direction
```

*where*

- The string `axis_name` is a name for this axis. This name must be unique to all other axes defined in the input file.

- The string `point` is the name of a point defined in the input file via a `DEFINE POINT` command line.

- The string `direction` is the name of a direction defined in the input file via a `DEFINE DIRECTION` command line.
2.1.7 Orientation

BEGIN ORIENTATION <string>orientation_name
SYSTEM = <string>RECTANGULAR|Z RECTANGULAR|CYLINDRICAL|SPHERICAL(RECTANGULAR)
#
POINT A = <real>global_ax <real>global_ay <real>global_az
POINT B = <real>global_bx <real>global_by <real>global_bz
#
ROTATION ABOUT <integer> 1|2|3(1) = <real>theta(0.0)
END [ORIENTATION <string>orientation_name]

The ORIENTATION command block is currently used in Presto to define a local coordinate system for output of shell stresses. In the future, the ORIENTATION command block will be used with other functionality in Presto.

A local coordinate system is defined at the particular location at which it is required. For example, suppose we want to define a local coordinate system for a shell element. This local coordinate system will be used for output of stresses in the element. For shell elements, the centroid of the element is where we want to define the local coordinates for output of stresses. When we use orientation with a shell element, the centroid of the shell element becomes the particular location at which we want to define a local coordinate system. (When we associate an orientation with a block of shell elements, the orientation will generate a local coordinate system for each element in the block.)

![Figure 2.2: Adjacent shell elements with nonaligned local coordinate systems](image)

To understand why we would want to specify the local coordinate system for shell elements, consider the example of two adjacent shell elements, as shown in Figure 2.2. A common notation system for a local coordinate system for a shell element defines the 1-axis as an axis lying in the shell; the 1-axis passes through the centroid of the shell. The 3-axis is normal to the shell at the centroid of the shell. The 2-axis is the cross-product of the 3-axis and 1-axis—\(3 \times 1\). The orientation of the 1-2-3 coordinate system for a shell element is determined by the connectivity for a shell element and the geometric location of the nodes. In Figure 2.2, the default local coordinate...
systems for the two elements do not align (the 1-axis in one element parallel to the 1-axis in the other element, the 2-axis in one element parallel to the 2-axis in the other element).

In general, for a shell element mesh, there is no guarantee that the default local system for one element will be reasonably aligned with its neighboring elements. The local coordinates for adjacent shell elements need to show a reasonable alignment to make it easier to interpret stress results, especially for graphical representations. Take the case of a cylindrical object modeled with shell elements. We might want the local 2-axis of each element to align with the cylindrical axis of the cylinder. We would want the local 1-axis of each element to be tangent to the cylinder and normal to the cylindrical axis. The ORIENTATION option gives us the ability to control the orientation for the local coordinate system for each element and align each one of these local coordinate systems so that it is easier to interpret stress information for shells.

The SYSTEM command line gives you several options for constructing a local coordinate system. The options on this command line are RECTANGULAR, Z RECTANGULAR, CYLINDRICAL, and SPHERICAL. The SYSTEM command line is optional. If you do not include a SYSTEM command line in the ORIENTATION command block, the default system is the RECTANGULAR system.

The ORIENTATION command actually generates two local coordinate systems. The first local system constructed at a particular location will always be a Cartesian system designated as $X'Y'Z'$. How this system is constructed depends on the choice for the SYSTEM option. Regardless of what system option you choose, the command lines POINT A and POINT B are required. The details of constructing a local coordinate system for each of the different SYSTEM options is described below.

**Figure 2.3: Rectangular coordinate system**

- **RECTANGULAR option**: The command line POINT A defines a point $a$ that lies on the $X'$-axis. The command line POINT B defines a point $b$ that lies in the $X'Y'$-plane (Figure 2.3). Let the coordinates of $a$ define a vector $\vec{A}$ and the coordinates of $b$ define a vector $\vec{B}$. The normalized value of $\vec{A}$, $\vec{A} / \| \vec{A} \|$, defines a unit vector along the $X'$-axis, which we denote as $\vec{X}'$. The normalized cross-product of $\vec{A} \times \vec{B}$ is a unit vector defining the $Z'$-axis, which we denote as $\vec{Z}'$. We can obtain a unit vector along the $Y'$-axis, $\vec{Y}'$, from a cross-product of $\vec{Z}'$ and $\vec{X}'$. The three unit vectors $\vec{X}'$, $\vec{Y}'$, and $\vec{Z}'$ give us our local coordinate system $X'Y'Z'$. 
CHAPTER 2. GENERAL COMMANDS

Figure 2.4: Z-Rectangular coordinate system.

- **Z RECTANGULAR** option: The command line **POINT A** defines a point \(a\) that lies on the \(Z'\)-axis. The command line **POINT B** defines a point \(b\) that lies in the \(X'Z'\)-plane (Figure 2.4). Let the coordinates of \(a\) define a vector \(\vec{A}\) and the coordinates of \(b\) define a vector \(\vec{B}\). The normalized value of \(\vec{A}, \vec{A}/\|\vec{A}\|\), defines a unit vector along the \(Z'\)-axis, which we denote as \(\vec{Z}'\). The normalized cross-product of \(\vec{A} \times \vec{B}\) is a unit vector defining the \(Y'\)-axis, which we denote as \(\vec{Y}'\). We can obtain a unit vector along the \(X'\)-axis, \(\vec{X}'\), from a cross-product of \(\vec{Y}'\) and \(\vec{Z}'\). The three unit vectors \(\vec{X}', \vec{Y}', \) and \(\vec{Z}'\) give us our local coordinate system \(X'Y'Z'\).

Figure 2.5: Cylindrical coordinate system.

- **CYLINDRICAL** option: The point \(a\) defined by the command line **POINT A** and the point \(b\) defined by the command line **POINT B** define a cylindrical axis (Figure 2.5). The local coordinate system always has the \(Z'\)-axis parallel to this cylindrical axis and in the direction from \(a\) to \(b\). The vector \(\vec{Z}'\) is a unit vector defining the \(Z'\)-axis. The \(X'\)-axis lies along a line that is normal to the cylindrical axis and passes through the origin of our local coordinate system. (e.g., if we are defining a local system for shell stress output, the origin of our local system is the centroid of the element.) The vector \(\vec{X}'\) is a unit vector defining the \(X'\)-axis. We can obtain the \(Y'\)-axis from the cross-product of the \(\vec{Z}'\) and \(\vec{X}'\) vectors. The three unit
vectors $\vec{X}', \vec{Y}',$ and $\vec{Z}'$ give us our local coordinate system $X'Y'Z'$.

![Spherical coordinate system](image)

**Figure 2.6: Spherical coordinate system.**

- **Spherical option**: The point $a$, from the **POINT A** command line, defines the center of a sphere. The point $b$, from the **POINT B** command line, defines a polar axis for the sphere. (See Figure 2.6.) The $X'$-axis lies along a line passing through the origin of the sphere, point $a$, and the origin of our local coordinate system. (e.g., if we are defining a local system for shell stress output, the origin of our local system is the centroid of the element.) The vector $\vec{X}'$ is a unit vector defining the $X'$-axis. A cross-product of the polar axis for the sphere and the vector $\vec{X}'$ gives the $\vec{Y}'$ vector. The vector $\vec{Y}'$ is a unit vector defining the $Y'$-axis. We can obtain the $Z'$-axis from the cross-product of the $\vec{X}'$ and $\vec{Y}'$ vectors. The three unit vectors $\vec{X}'$, $\vec{Y}'$, and $\vec{Z}'$ give us our local coordinate system $X'Y'Z'$.

The second local coordinate system constructed at a particular location is defined by use of the **ROTATION ABOUT** command line. This second local coordinate system is always a Cartesian system that is designated as $X''Y''Z''$. The **ROTATION ABOUT** command line has the following form:

$$\text{ROTATION ABOUT } 1|2|3(1) = \text{<real>theta}(0.0)$$

The second local coordinate system, $X''Y''Z''$, is obtained by specifying some rotation, the theta parameter, about an axis, which is specified with an integer value of 1, 2, or 3. (The 1, 2, and 3 notation used in this command line should not be confused with the axes of the 1-2-3 local coordinate system. The 1 in this command line implies rotation about $X'$, the 2 implies rotation about $Y'$, and the 3 implies rotation about $Z'$.) The parameter theta has units of degrees. The manner in which the $X''Y''Z''$ is generated is as follows:

- **Rotation about the $X'$-axis** (**ROTATION ABOUT 1**: If the **ROTATION ABOUT** command line uses a value of 1, then the $X''Y''Z''$ coordinate system is obtained by a transformation that rotates the $X'Y'Z'$ coordinate system by theta degrees about the $X'$-axis. The local origin for $X''Y''Z''$ is the same as that for $X'Y'Z'$. For shell elements, the $Y''$-axis is projected onto the shell element to form the local 1-axis for the shell element. The 3-axis is the normal to the shell at the centroid. The 2-axis is the cross-product of the 3-axis and the 1-axis.)
For this case, \texttt{ROTATION ABOUT 1}, of the \texttt{ROTATION ABOUT} command line, an example is shown in Figure 2.7. After the rotation about the \textit{X}'-axis, the \textit{X}' and \textit{X}'' axes coincide. Both the \textit{Y}'' and \textit{Z}'' axes are rotated and both axes remain in the original \textit{Y}'\textit{Z}'-plane. Similar patterns exist for the cases of \texttt{ROTATION ABOUT 2} and \texttt{ROTATION ABOUT 3}.

- **Rotation about the \textit{Y}'-axis (\texttt{ROTATION ABOUT 2}):** If the \texttt{ROTATION ABOUT} command line uses a value of 2, then the \textit{X}'\textit{Y}''\textit{Z}'' coordinate system is obtained by a transformation that rotates the \textit{X}'\textit{Y}'\textit{Z}' coordinate system by \texttt{theta} degrees about the \textit{Y}'-axis. The local origin for \textit{X}'\textit{Y}''\textit{Z}'' is the same as that for \textit{X}'\textit{Y}'\textit{Z}'. For shell elements, the \textit{Z}''-axis is projected onto the shell element to form the local 1-axis for the shell element. The 3-axis is the normal to the shell at the centroid. The 2-axis is the cross-product of the 3-axis and the 1-axis.

- **Rotation about the \textit{Z}'-axis (\texttt{ROTATION ABOUT 3}):** If the \texttt{ROTATION ABOUT} command line uses a value of 3, then the \textit{X}'\textit{Y}''\textit{Z}'' coordinate system is obtained by a transformation that rotates the \textit{X}'\textit{Y}'\textit{Z}' coordinate system by \texttt{theta} degrees about the \textit{Z}'-axis. The local origin for \textit{X}'\textit{Y}''\textit{Z}'' is the same as that for \textit{X}'\textit{Y}'\textit{Z}'. For shell elements, the \textit{X}''-axis is projected onto the shell element to form the local 1-axis for the shell element. The 3-axis is the normal to the shell at the centroid. The 2-axis is the cross-product of the 3-axis and the 1-axis.

If the \texttt{ROTATION ABOUT} command line is not included in the \texttt{ORIENTATION} command block, the \textit{X}'\textit{Y}''\textit{Z}'' coordinate system is generated with a rotation about the \textit{X}'-axis of zero degree, e.g., the \texttt{ROTATION ABOUT} command line defaults to a value of 1 with the value of the parameter \texttt{theta} set to zero 0.0. The default values imply that the \textit{Y}''-axis is projected on the shell element to determine the local 1-axis.
2.2 Procedure and Region

The Presto procedure scope is nested within the domain scope, and the Presto region scope is nested within the procedure scope (see Section 1.2 for more information about scope). To create the scopes for the Presto procedure and Presto region, use the following commands:

```plaintext
BEGIN PRESTO PROCEDURE <string>presto_procedure_name
# TIME CONTROL command block
BEGIN PRESTO REGION <string>presto_region_name
# command blocks and command lines that appear in the region scope
END [PRESTO REGION <string>presto_region_name]
END [PRESTO PROCEDURE <string>presto_procedure_name]
```

The `TIME CONTROL` command block also appears within the `PRESTO PROCEDURE` command block but outside of the `PRESTO REGION` command block. These three command blocks (procedure, time control, and region) are discussed below.

Many command blocks and command lines fall within the region scope. These command blocks and command lines are described in other sections of this document.

2.2.1 Procedure

The analysis time, from the initial time to the termination time, is controlled within the procedure scope defined by the `PRESTO PROCEDURE` command block. The command block begins with an input line of the form:

```plaintext
BEGIN PRESTO PROCEDURE <string>presto_procedure_name
```

and is terminated with an input line of the following form:

```plaintext
END [PRESTO PROCEDURE <string>presto_procedure_name]
```

The string `presto_procedure_name` is the name for the Presto procedure.

2.2.2 Time Control

Within the procedure scope, there is a `TIME CONTROL` command block. This command block lets the user set the initial time and the termination time for an analysis. This block also allows the user to control the size of the time step.

Because Presto is an explicit, transient dynamics code, it must run at a time step that is less than the critical time for the problem at any given instant. Typically, this global critical time step is based
on a critical time step estimate calculated for each element. With the \texttt{TIME CONTROL} command block, the user can set an initial time step, scale the element-based time step estimate, and control the growth of the element-based estimate for the critical time step.

In addition to the element-based method for estimating the critical time step, Presto offers other methods for estimating the critical time step. One approach for estimating the critical time step is to calculate the maximum eigenvalue for the model. There are two methods for calculating the maximum eigenvalue: the Lanczos method and the power method. A second approach for estimating the critical time step is to use a node-based method. The command blocks for implementing these various methods (maximum eigenvalue calculation and node-based) are in the region scope. There is also a mass-scaling technique that will influence the magnitude of the critical time step. If you use the mass-scaling technique, you must use the node-based method to obtain a critical time step estimate.

The estimation of the time step is a key part of any Presto analysis. Time step determination and control is discussed in detail in Chapter 3 of this document. The \texttt{TIME CONTROL} command block with its associated command lines are described in detail in Chapter 3. Consult Chapter 3 to determine how to specify command lines associated with the \texttt{TIME CONTROL} command block and how the \texttt{TIME CONTROL} command block fits into the overall scheme for time step control in Presto. Also consult with Chapter 3 to learn about the other methods for estimating the critical time step and the mass-scaling technique.

### 2.2.3 Region

Individual time steps are controlled within the region scope. The region scope is defined by a \texttt{PRESTO REGION} command block that begins with an input line of the form

\begin{verbatim}
BEGIN PRESTO REGION <string>presto_region_name
\end{verbatim}

and is terminated with an input line of the following form:

\begin{verbatim}
END [PRESTO REGION <string>presto_region_name]
\end{verbatim}

The string \texttt{presto_region_name} is the name for the Presto region.

The region, as indicated previously, determines what happens at each time step. In the procedure, we set the begin time and end time for the analysis. Time is incremented in the region. It is in the region where we set information about what occurs at various time steps. The output of results, for example, is set by command blocks in the region. If we want results output at certain times or certain steps in the analysis, this information is set in command blocks in the region. The region also contains command blocks for the boundary conditions. A boundary condition can have a time-varying component. The region determines the value of the component for the current time step.

Two of the major types of command blocks, those for results output and boundary conditions, have already been mentioned. Other major types of command blocks in the region are those for restart control and contact. The region is also where the user selects the analysis model (finite element mesh).
The region makes use of information in the procedure and the domain. For example, the specific element type used for an element block in the analysis model is defined in the domain. This information about the element type is collected into an analysis model. The region then references this analysis model. As another example, the boundary condition command blocks can reference a function. The function will be defined in the domain.
2.3 Use Finite Element Model

```
USE FINITE ELEMENT MODEL <string>model_name
```

The model specification occurs within the region scope. To specify the model (finite element mesh), use this command line. The string `model_name` must match a name used in a `FINITE ELEMENT MODEL` command block described in Section 5.1. If one of these command blocks uses the name `penetrator` in the command-block line and this is the model we wish to use in the region scope, then we would enter the command line as follows:

```
USE FINITE ELEMENT MODEL penetrator
```
2.4 Error Estimation

Presto incorporates a number of user-defined error estimators. These error estimators can be used to help assess the quality of the solution as the mesh evolves through time. A selected error estimator will calculate the specified error metric on every supported element of the mesh.

The following sections describe the use of the error estimators in Presto.

2.4.1 Error Estimation Controller

BEGIN ERROR ESTIMATION CONTROLLER <string>err_name
ERROR ESTIMATOR = <string>DISTORTION
COMPUTE METRIC = <string>ASPECT_RATIO|SOLID_ANGLE|PERIMETER_RATIO
COMPUTE STEP INTERVAL = <integer>step_int
COMPUTE AT OUTPUT
END [ERROR ESTIMATION CONTROLLER <string>err_name]

The full definition of an error estimation method is given in an ERROR ESTIMATION CONTROLLER command block. This block must be defined in the domain scope, i.e., at the same level as material models and functions. Note that there can be multiple ERROR ESTIMATION CONTROLLER command blocks defined in the domain scope. The user-defined error estimation methods are available for use within any Presto region through inclusion of the USE ERROR ESTIMATION CONTROLLER command line in the region scope (see Section 2.4.2).

The command block begins with an input line of the form

BEGIN ERROR ESTIMATION CONTROLLER <string>err_name

and ends with an input line of the following form:

END [ERROR ESTIMATION CONTROLLER <string>err_name]

Here, err_name is a user-selected name for the ERROR ESTIMATION CONTROLLER command block. The command lines within the block define what type of error metric to calculate, how to calculate the metric, and when to calculate the metric. The valid commands within this block are described next in Section 2.4.1.1 through Section 2.4.1.3.

2.4.1.1 Error Estimator Class

ERROR ESTIMATOR = <string>DISTORTION

This command line specifies the type of error metric to calculate. Currently, there is only a single class of error estimators available to Presto, the DISTORTION class. The distortion error metric measures the distortion of mesh elements as they deform and distort through time. If an element becomes inverted, the analysis will abort. As an element nears inversion, the solution generally becomes poor. The distortion error metric measures how close an element is to inversion.
2.4.1.2 Distortion Metrics

\text{COMPUTE METRIC} = \text{<string>ASPECT_RATIO|SOLID_ANGLE|PERIMETER_RATIO}

There are three formulations for error metrics, or error estimates, available within the distortion class: aspect ratio, solid angle, and perimeter ratio. Selection of a metric (or metrics) may be specified by the \text{COMPUTE METRIC} command line.

- If the \text{ASPECT_RATIO} option is specified, the aspect ratio is computed for tetrahedral elements. A perfect equilateral tetrahedron has an aspect ratio of 1.0. A degenerate zero-volume tetrahedron has an aspect ratio of zero. An inverted tetrahedron has a negative aspect ratio. A very thin element can have very large aspect ratios. The \text{ASPECT_RATIO} option will only work on tetrahedral elements.

- If the \text{SOLID_ANGLE} option is specified, the minimal or maximal angle between edges of an element is computed. The optimal solid angle for tetrahedrons and triangles is 60 degrees; for hexahedrons and quadrilaterals, it is 90 degrees. An element in which all angles are optimal has an error metric of 1, whereas a degenerate element has an error metric of 0 and an inverted element has a negative solid angle. Severely distorted or twisted elements will have poor (near 0) solid angles. The \text{SOLID_ANGLE} option operates on any two-dimensional or three-dimensional element type in Presto.

- If the \text{PERIMETER_RATIO} option is specified, the ratio of the deformed perimeter of an element to the undeformed perimeter of the element is computed. If we take the ratio of the perimeter of an undeformed element to the perimeter of the undeformed element, obviously, we will get a value of 1. If, however, we take the ratio of the perimeter of a deformed element to the perimeter of the element in the undeformed state, the perimeter ratio for the deformed element may have a value either larger or smaller than 1, depending on the amount of deformation. The \text{PERIMETER_RATIO} option will only work on three- and four-node two-dimensional elements.

If you want to examine two or three error estimates on the same mesh, you can include any combination of \text{ASPECT_RATIO}, \text{SOLID_ANGLE}, and \text{PERIMETER_RATIO} in the command line. A multiple error estimate request produces all the results that are applicable based on the range of element types. For example, if you want to examine both the aspect ratio and the solid angle on a mesh, you could include both \text{ASPECT_RATIO} and \text{SOLID_ANGLE} in the \text{COMPUTE METRIC} command line. If the mesh consisted solely of tetrahedral and hexahedral elements, an aspect ratio and a solid angle would be computed for all the tetrahedral elements in the mesh; only a solid angle would be computed for the hexahedral elements. The results are automatically stored in output variables when computed, one variable for each metric.

\text{ASPECT_RATIO}, \text{SOLID_ANGLE}, and \text{PERIMETER_RATIO} are treated as element variables. Thus, you can request that the results computed for any of the specified variables be output from Presto by specifying an \text{ELEMENT VARIABLES} command line (Section 8.1.1.4) in the \text{RESULTS OUTPUT} command block (Section 8.1.1) for each metric for which the results are of interest. Suppose you
have specified the ASPECT_RATIO option, you can write the values for the aspect ratio for the appropriate elements by including a command line of the form in a RESULTS OUTPUT command block (see Section 8.1.1 for more details about obtaining results output):

\[
\text{ELEMENT VARIABLES = ASPECT\_RATIO as aspect}
\]

In the above command line, the element variable ASPECT\_RATIO is assigned the name aspect on the results output file.

The three distortion metrics can also be used for element death (Section 5.5). As an example, suppose you have specified the SOLID\_ANGLE option. You can use the solid angle value of an element as an element death criterion by including the following command line:

\[
\text{CRITERION IS ELEMENT VALUE OF SOLID\_ANGLE < 30.0}
\]

Any element with a solid angle value less than 30.0 degrees will be killed. For more information about the use of the distortion metrics as an element variable for element death, see Section 5.5.2.2.

2.4.1.3 Utilities

\[
\begin{align*}
\text{COMPUTE STEP INTERVAL} & = \text{<integer>}\text{step\_int} \\
\text{COMPUTE AT OUTPUT}
\end{align*}
\]

An ERROR ESTIMATION CONTROLLER command block may contain one or both of the above command lines to control the frequency and output of error metrics.

The COMPUTE STEP INTERVAL command line specifies how often the error metrics are computed. The metric will be computed every step\_int time steps.

The COMPUTE AT OUTPUT command line specifies that error estimators should only be computed immediately prior to results output.

If both COMPUTE STEP INTERVAL and COMPUTE AT OUTPUT are specified, the error would be computed every \(n\) time steps. Additionally, the error would be computed immediately prior to writing an output file to ensure that output values are correct for visualization. Specifying both command lines is reasonable in many analyses. For example, a user may wish to view the correct current error estimate on the mesh when it is output and use the error estimate to compute element death. The COMPUTE STEP INTERVAL command line can be used to ensure the error estimator is updated sufficiently often to steer the calculation, but not so often as to incur a major computational cost due to error estimation.

2.4.2 Use Error Estimation Controller

\[
\text{USE ERROR ESTIMATION CONTROLLER <string>err\_name}
\]

The activation of an error estimation controller occurs within the region scope. To specify the controller, use this command line. The string err\_name must match a name used in an ERROR
ESTIMATION CONTROLLER command block described in Section 2.4.1. If one of these command blocks uses the name estim1 in the command-block line and this is the controller we wish to use in the region, then we would enter the command line as follows:

```
USE ERROR ESTIMATION CONTROLLER estim1
```

Each Presto region may use at most one of the defined error estimation methods via the USE ERROR ESTIMATION CONTROLLER command line.
The **ACTIVE PERIODS** command line can be used to activate or deactivate functionality in the code at various points during an analysis. This functionality can include such things as boundary conditions, element blocks, and user subroutines. In the command line, the string list `period_names` is a list of the time periods defined in **TIME STEPPING BLOCK** command blocks (see Section 3.1) during which the particular functionality is considered to be active. Each such `period_name` must match a name used in a **TIME STEPPING BLOCK** command block, e.g., `time_block_name`. Each defined time period runs from that period’s start time to the next period’s start time. Note that if the **ACTIVE PERIODS** command line is present, the functionality will be treated as inactive for any time periods that are not listed. If this command line is absent, then by default, the functionality is active during all time periods. Various other command blocks in Presto will indicate whether they can be used with the **ACTIVE PERIODS** command line.
Chapter 3

Time Step Control in Presto

This chapter discusses time control in Presto. We begin with a broad overview of time control in Presto and then describe the options that are available to users for time control.

The user initiates time control in Presto by setting a start time and a termination time for an analysis. The analysis is typically carried out with a large number of time steps, with each time step being much smaller than the analysis time. Because Presto is an explicit, transient dynamics code, a time step must be less than some critical value. Presto has a number of methods for computing an estimate for the critical time step. These methods are discussed in detail in this chapter.

The primary time control uses a TIME CONTROL command block that appears in the procedure scope. Use of the TIME CONTROL command block gives the user, by default, access to an element-based method for estimating the critical time step. The user can access three other methods for estimating the critical time step by using specific command blocks that are placed in the region scope. These other methods tend to give better (larger) estimates for the critical time step. In addition, Presto has a technique for adjusting the time step that is known as mass scaling.

Section 3.1 describes the TIME CONTROL command block. In Section 3.2 we discuss the other methods for estimating the critical time step. One approach for improving this estimate is to compute the maximum eigenvalue for a problem. Two methods for computing the maximum eigenvalue are available in Presto: the Lanczos method and the power method. Section 3.2.1 discusses the Lanczos method; Section 3.2.1.5 describes the command block required to implement the Lanczos method. Section 3.2.2 discusses the power method; Section 3.2.2.5 describes the command block required to implement the power method. Another approach for improving the time step estimate relies on a node-based estimate. Section 3.2.3 discusses the node-based method; Section 3.2.3.1 describes the command block required to implement the node-based method. You should read the introductory material for the maximum eigenvalue calculation methods and the node-based method and understand this material thoroughly before you attempt to use these methods. Although these other methods give larger time step estimates than the element-based method, they may not result in a net reduction of central processor unit (CPU) time for an analysis unless they are used properly. In those sections dealing with these other methods, we discuss how to use these methods in a cost-effective manner. Finally, in Section 3.2.3 we describe the technique of mass scaling. Mass scaling is a much different approach for adjusting the time step when compared
to the methods (element-, node-, maximum eigenvalue-based) we have just been discussing. The command block for mass scaling is in the region scope. Importantly, the mass-scaling technique requires that the node-based method of estimating the critical time step also be used.

3.1 Procedure Time Control

As indicated previously, the primary time control in Presto uses a \texttt{TIME CONTROL} command block in the procedure scope. The user sets the start time and the termination time for the analysis in the \texttt{TIME CONTROL} command block. For reference purposes, the general layout of the command block is as follows:

\begin{verbatim}
BEGIN TIME CONTROL
  BEGIN TIME STEPPING BLOCK <string>time_block_name
    START TIME = <real>start_time_value
    BEGIN PARAMETERS FOR PRESTO REGION <string>region_name
      INITIAL TIME STEP = <real>initial_time_step_value
      TIME STEP SCALE FACTOR =
        <real>time_step_scale_factor(1.0)
      TIME STEP INCREASE FACTOR =
        <real>time_step_increase_factor(1.1)
      STEP INTERVAL = <integer>nsteps(100)
    END [PARAMETERS FOR PRESTO REGION <string>region_name]
  END [TIME STEPPING BLOCK <string>time_block_name]
# Second TIME STEPPING BLOCK command block
# would be placed here, as applicable.
# Additional TIME STEPPING BLOCK command blocks
# would be placed here, as applicable.
# Last TIME STEPPING BLOCK command block
# would be placed here, as applicable.
  TERMINATION TIME = <real>termination_time
END [TIME CONTROL]
\end{verbatim}

The analysis time, as demonstrated above, can be subdivided into a number of time blocks, i.e., \texttt{TIME STEPPING BLOCK} command blocks. If the total analysis time is from time 0 to time $T$ and there are three blocks, then the first block is defined from time 0 to time $t_1$, the second block is defined from time $t_1$ to time $t_2$, and the third block is defined from time $t_2$ to time $T$. (The times $t_1$ and $t_2$ are set by the user.) If we sum all the times for each block, the sum will be $T$. The different time periods defined by each block can be referenced so that we can turn certain functionality on or off throughout an analysis. For example, we may want to have a certain boundary condition turned off during our first time period and activated for the second time period. (Most analyses require only one block.) Use the \texttt{ACTIVE PERIODS} command line described in Section 2.5 to activate and deactivate functionality.
By default, Presto relies on the element-based critical time step estimate. At every time step, an element-based calculation is performed to determine a critical time step. You have some control over the actual time step that is used by employing one of two techniques. We discuss these two techniques in the following paragraphs. The specific command lines for using these techniques are described in Section 3.1.1.

With the first technique, you can set an initial time step that is smaller than the element-based critical time step estimate. Presto will start the analysis by using your initial time step value instead of the element-based critical time step estimate (as long as your value is less than the element-based critical time step estimate). You can then control the rate at which the time step increases from your initial value. This technique is employed by using the `TIME STEP INCREASE FACTOR` command line as follows:

- If you set a time step increase factor equal to 1, then the initial value you specified will be used throughout the analysis (provided that the initial time step is never smaller than the element-based critical time step estimate throughout the computations).

- If you set a time step increase factor to some value greater than 1, the time step will grow (from the initial value) at each time step until it reaches the value of the element-based critical time step estimate. From then on, the element-based critical time step estimate will essentially control the time step.

With the second technique, you can manipulate the element-based estimate with either a scale factor or a time step increase factor. This technique is employed by using the `TIME STEP SCALE FACTOR` command line or the `TIME STEP INCREASE FACTOR` command line as follows:

- The element-based estimate for the critical time step is usually smaller than some maximum theoretical value for your model. It may therefore be possible to scale the element-based critical time step estimate by some factor greater than 1. (Your scaled value must remain below the theoretical maximum limit, however. We discuss ways to obtain a critical time step close to the theoretical maximum in later sections of this chapter.)

- If there are stability problems with a particular problem, it may be necessary to scale the element-based estimate with a factor less than 1.

- You can also control the rate at which the time step can increase for an analysis. By specifying a time step increase factor, you can limit the increase in the size of the time step so that it does not increase too rapidly from one step to the next. For certain problems, the element-based critical time step estimate may increase rapidly from one step to the next. Limiting the increase in the size of the time step may enable some problems to run in a more stable fashion.

Now that we have presented an overview of the functionality in the `TIME CONTROL` command block, we will discuss the actual command lines.
3.1.1 Command Blocks for Time Control and Time Stepping

BEGIN TIME CONTROL
BEGIN TIME STEPPING BLOCK <string>time_block_name
START TIME = <real>start_time_value
BEGIN PARAMETERS FOR PRESTO REGION <string>region_name
#
# Time control parameters specific to PRESTO
# are set in this command block.
#
END [PARAMETERS FOR PRESTO REGION <string>region_name]
END [TIME STEPPING BLOCK <string>time_block_name]
TERMINATION TIME = <real>termination_time
END [TIME CONTROL]

Presto time control resides in a TIME CONTROL command block. The command block begins with an input line of the form

BEGIN TIME CONTROL

and terminates with an input line of the following form:

END [TIME CONTROL]

Within the TIME CONTROL command block, a number of TIME STEPPING BLOCK command blocks can be defined. Each TIME STEPPING BLOCK command block contains the time at which the time stepping starts and a number of parameters that set time-related values for the analysis. Each TIME STEPPING BLOCK command block terminates at the start time of the following command block. The start times for the TIME STEPPING BLOCK command blocks must be in increasing order. Otherwise, an error will be generated by Presto. (The example in Section 3.1.6 shows the overall structure of the TIME CONTROL command block.)

In the above input lines, the values are as follows:

- The string time_block_name is a name for the TIME STEPPING BLOCK command block. This name must be unique to the other command blocks of this type. The string time_block_name can be referenced on an ACTIVE PERIODS command line to activate and deactivate functionality (see Section 2.5).

- The real value start_time_value is the start time for this TIME STEPPING BLOCK command block. Values set by the block apply from the start time for this block until the next start time or the termination time.

- The string region_name is the name of the Presto region affected by the parameters (see Section 2.2).

The termination time for the analysis is given by the following command line:

TERMINATION TIME = <real>termination_time
Here, termination_time is the time at which the analysis will stop. The TERMINATION TIME command line appears inside the TIME CONTROL command block but outside of any TIME STEPPING BLOCK command block.

The TERMINATION TIME command line can appear before the first TIME STEPPING BLOCK command block or after the last TIME STEPPING BLOCK command block. Note that it is permissible to have TIME STEPPING BLOCK command blocks with start times after the termination time; in this case, those command blocks that have start times after the termination time are not executed. Only one TERMINATION TIME command line can appear in the TIME CONTROL command block. If more than one of these command lines appears, Presto gives an error.

Nested inside the TIME STEPPING BLOCK command block is a PARAMETERS FOR PRESTO REGION command block containing parameters that control the time stepping.

BEGIN PARAMETERS FOR PRESTO REGION <string>region_name
  INITIAL TIME STEP = <real>initial_time_step_value
  TIME STEP SCALE FACTOR = <real>time_step_scale_factor(1.0)
  TIME STEP INCREASE FACTOR = <real>time_step_increase_factor(1.1)
  STEP INTERVAL = <integer>nsteps(100)
END [PARAMETERS FOR PRESTO REGION <string>region_name]

These parameters are specific to a Presto analysis.

The command block begins with an input line of the form

BEGIN PARAMETERS FOR PRESTO REGION <string>region_name

and is terminated with an input line of the following form:

END [PARAMETERS FOR PRESTO REGION <string>region_name]

As noted previously, the string region_name is the name of the Presto region affected by the parameters. The command lines nested inside the PARAMETERS FOR PRESTO REGION command block are described next. It should be noted that certain of these command lines will be ignored when either of the maximum-eigenvalue methods or the node-based method is used to estimate the critical time step. The discussions of the command blocks associated with these methods indicate whether or not these command lines are pertinent.

### 3.1.2 Initial Time Step

INITIAL TIME STEP = <real>initial_time_step_value

By default, Presto computes a critical time step for the analysis and uses this value as the initial time step. To directly specify a different initial time step, use the INITIAL TIME STEP command line, where initial_time_step_value is the size of the initial time step. This command line is only valid if it is in the first TIME STEPPING BLOCK command block in the problem.
The value for the initial time step will overwrite the calculated value for the critical time step. If you specify an initial time step that is larger than the critical time step, the time step is set to the value of the calculated critical time step.

### 3.1.3 Time Step Scale Factor

\[
\text{TIME STEP SCALE FACTOR} = <\text{real}> \text{time_step_scale_factor}(1.0)
\]

During the element computations, Presto computes a minimum time step required for stability of the computation (the critical time step). Using the \text{TIME STEP SCALE FACTOR} command line, you can provide a scale factor to modify the critical time step. Note that a value greater than 1.0 for \text{time_step_scale_factor} will cause the time step to be greater than the computed critical time step, and thus the problem may become unstable. By default, the scale factor is 1.0.

### 3.1.4 Time Step Increase Factor

\[
\text{TIME STEP INCREASE FACTOR} = <\text{real}> \text{time_step_increase_factor}(1.1)
\]

During an analysis, the computed critical time step may change as elements deform, are killed, and so forth. By using the \text{TIME STEP INCREASE FACTOR} command line, you can limit the amount that the time step can increase between two adjacent time steps. The value \text{time_step_increase_factor} is a factor that multiplies the previous time step. The current time step can be no larger than the product of the previous time step and the scale factor.

Note that an increase factor less than 1.0 will cause the time step to continuously decrease. The default value for this factor is 1.1, i.e., a time step cannot be more than 1.1 times the previous step.

### 3.1.5 Step Interval

\[
\text{STEP INTERVAL} = <\text{integer}> \text{nsteps}(100)
\]

Presto can output data about the current time step, the current internal and external energy, and the kinetic energy throughout an analysis. The \text{STEP INTERVAL} command line controls the frequency of this output, where \text{nsteps} is the number of time steps between output. The default value for \text{nsteps} is 100.

The output at any given step (read from left to right) is

- step number,
- time,
- time step,
3.1. PROCEDURE TIME CONTROL

- global element identifier for element controlling time step
- kinetic energy,
- internal energy,
- external energy (work done on boundary),
- error in energy balance,
- hour glass energy
- cpu time, and
- wall clock time.

The time is at the current time, step \( n \), and the time increment is the previous time step increment from step \( n - 1 \) to step \( n \).

The error in the energy balance is computed from the following relation:

\[
\text{energy balance error} = \frac{(\text{kinetic energy} + \text{internal energy} - \text{external energy})}{\text{external energy}} \times 100
\]

The above expression gives a percent error for the energy balance.

3.1.6 Example

The following is a simple example of a TIME CONTROL command block:

```
BEGIN TIME CONTROL
  BEGIN TIME STEPPING BLOCK p1
    START TIME = 0.0
    BEGIN PARAMETERS FOR PRESTO REGION presto_region
      INITIAL TIME STEP = 1.0e-6
      STEP INTERVAL = 50
    END
  END

  BEGIN TIME STEPPING BLOCK p2
    START TIME = 0.5e-3
    BEGIN PARAMETERS FOR PRESTO REGION presto_region
      TIME STEP SCALE FACTOR = 0.9
      TIME STEP INCREASE FACTOR = 1.5
      STEP INTERVAL = 10
    END
  END

  TERMINATION TIME = 1.0e-3
END
```
The first TIME STEPPING BLOCK, p1, begins at time 0.0, the initial start time, and terminates at time $0.5 \times 10^{-3}$. The second TIME STEPPING BLOCK, p2, begins at time $0.5 \times 10^{-3}$ and terminates at time $1.0 \times 10^{-3}$, which is the time listed on the TERMINATION TIME command line. The TIME STEPPING BLOCK names p1 and p2 can be referenced by ACTIVE PERIODS command lines described in Section 2.5 to activate and deactivate functionality.
3.2 Other Critical Time Step Methods

Currently, there are four methods for calculating a critical time step for Presto. First, there is the traditional element-based method. We know that, in general, the element-based time step in Presto can give a fairly conservative estimate for the time step. Second, there is a node-based method for giving a critical time step estimate. Depending on the problem, the node-based method may or may not give an estimate for the critical time step that approaches the theoretical maximum value for a particular model. Although the node-based method can give a larger critical time step estimate than the element-based method, the node-based estimate may still be significantly lower than the maximum theoretical time step for a problem. Finally, there are two methods that use an estimate for the maximum eigenvalue to obtain an estimate for the critical time step. From the maximum eigenvalue, it is possible to derive the theoretical maximum critical time step for a problem via the formula

$$
\Delta t_{crit} = \frac{2.0}{\sqrt{\theta_{max}}},
$$

where $\Delta t_{crit}$ is the critical time step and $\theta_{max}$ is the maximum eigenvalue. The two methods employed in Presto to give an estimate for the maximum eigenvalue are the Lanczos method and the power method. The Lanczos method can give an accurate estimate of the maximum eigenvalue for a problem using a very small number of Lanczos vectors compared to the total number of degrees of freedom in a problem. The power method uses a simple iterative process to obtain an estimate for the maximum eigenvalue. The power method is not as powerful a mathematical technique as the Lanczos method for obtaining a maximum eigenvalue estimate. However, it does present another viable option for obtaining a maximum eigenvalue estimate for certain problems and has therefore been included as another method for obtaining the maximum eigenvalue estimate.

The use of a critical time step from the node-based method or a method based on the maximum eigenvalue estimate is desirable because the larger critical time steps produced by these methods (compared to the element-based method) reduce CPU time. Both methods, however, are not cost effective if they are called every time step to give a critical time step estimate. The cost of doing one node-based estimate or one maximum eigenvalue estimate for the critical time step will not offset the cost benefit of the increase to the critical time step (compared to the element-based time step estimate) over a single time step. Hence, there must be some scheme for

- calling these methods only periodically throughout a calculation and
- maintaining a larger estimate (than the element-based estimate) for the critical time step in between these calls

if we are to gain a net benefit from the increase in the critical time step these methods can produce.

If you want to use the maximum eigenvalue estimate for calculating the critical time step and your problem has long periods with a relatively stable time step estimate, the Lanczos method for calculating the maximum eigenvalue will be the preferred method to use. If you have a problem for which the changes in the time step should be monitored more frequently, the power method will be better suited for this problem than the Lanczos method. The preferred use for each of these
two different eigenvalue methods will become obvious as you read the background material for these two methods in Section 3.2.1 and Section 3.2.2. Both the Lanczos method and the power method require the use of a variety of control parameters. For some of these control parameters, techniques have been devised to automatically calculate values for these parameters in what should be a robust and reliable method for a wide range of problems. Other parameters are defaulted to values that will optimize the use of a particular eigenvalue calculation method (Lanczos method or power method) with the type of problems that best suit the method that is employed. The default values for these control parameters may change as we gain more experience in using the Lanczos method and the power method.

Detailed discussions of the Lanczos method, the power method, and the node-based method follow. There are many similarities in the implementation of the Lanczos method and the power method.

### 3.2.1 Lanczos Method

The Lanczos method, as implemented in Presto, is outlined here so that certain aspects of it can be referenced in subsequent parts of this chapter. In the following set of equations, $K_T$ is a tangent stiffness matrix, $M$ is the mass matrix, and $r_0$ is an arbitrary starting vector.

**Initialize**

\[
\begin{align*}
q_0 &= 0 \\
\beta &= ([r_0]^T M^{-1} r_0)^{1/2} \\
q_1 &= r_0/\beta \\
p_1 &= Mq_1
\end{align*}
\]

for $j = 1, n$

\[
\begin{align*}
\hat{r}_j &= K_T p_j \\
\hat{r}_j &= \hat{r}_j - q_{j-1}\beta_j \\
\alpha_j &= [q_j]^T M^{-1} \hat{r}_j = [p_j]^T r_j \\
r_j &= \hat{r}_j - q_j\alpha_j \\
p_j &= M^{-1} r_j \\
\beta_{j+1} &= ([r_j]^T M^{-1} r_j)^{1/2} = ([p_j]^T r_j)^{1/2}
\end{align*}
\]

if enough vectors, terminate loop

\[
\begin{align*}
q_{j+1} &= r_j/\beta_{j+1} \\
p_{j+1} &= p_j/\beta_{j+1}
\end{align*}
\]

end

The details for this form of the Lanczos method are described in Reference 1. Notice that the Lanczos method is an iterative method. If we use the Lanczos method in a code like Presto to compute the maximum eigenvalue for a particular finite element model, the number of iterations
3.2. OTHER CRITICAL TIME STEP METHODS

required to give a good estimate for the maximum eigenvalue will depend on the size of the finite element model (the number of nodes and elements), the types of elements in the model, and the material types and material properties used in the model.

The maximum eigenvalue for a particular finite element model gives us the largest estimate we can obtain for the critical time step. Hence, the time step estimate derived from the maximum eigenvalue is our “best” estimate for the critical time step. The estimate for the critical time step based on the maximum eigenvalue can be significantly larger than an element-based time step estimate. However, computing the critical time step (for a given time step) with the Lanczos method is more expensive than computing the critical time step with element-based calculations. Over one time step, it is not possible to recoup the cost of the Lanczos calculations with the increase in the size of the time step over the element-based estimate. Using the Lanczos method for estimating the critical time step in an explicit, transient dynamics code requires a methodology that effectively addresses the computational costs. The following sections outline a cost-effective approach to using the Lanczos method in an explicit, transient dynamics code.

3.2.1.1 Lanczos Method with Constant Time Steps

To explain how to use the Lanczos method in a cost-efficient manner, we must first establish the computational cost of using the Lanczos method. As indicated previously, computing the maximum eigenvalue for a finite element model requires some number of iterations (each iteration in the Lanczos method produces a Lanczos vector) to obtain a good estimate for the maximum eigenvalue. The cost of an iteration (Lanczos vector) is approximately the cost of an internal force calculation. Notice, in preceding equations for the Lanczos method, that the Lanczos method requires the product of the tangent stiffness matrix $K_T$ with a vector $p$. In Presto, we do not construct a tangent stiffness matrix. Instead, we simply provide the vector $p$ for the internal force calculations. The internal force calculations give us the desired matrix $\times$ vector product of $K_T p$.

Over a given time step, the cost of an internal force calculation is the major computational cost. (This assumes no contact. The addition of contact introduces another computationally expensive process into a time step. For our initial discussion, we ignore the cost of contact.) In order to use the Lanczos method to get a critical time step estimate, one has to call the Lanczos method for some given time step. If the Lanczos method made $n$ iterations to get a good estimate for the maximum eigenvalue, then the overall cost of the time step would be approximately $n + 1$ times the cost of the internal force calculation. The cost of the time step would be the $n$ internal force calculations for Lanczos and the actual internal force calculation to advance the time step. If $n$ is 20 (a minimum for typical problems), the cost of the time step becomes 21 times the cost of the internal force calculation. The critical time step estimate based on the maximum eigenvalue would have to be at least 21 times greater than the element-based critical time step to recoup the cost of the maximum eigenvalue calculation. A typical value for the critical time step estimate based on the maximum value is more in the range of 1.1 to 2.0 times the element-based critical time step estimate. Obviously, the Lanczos method is much too expensive to call at every time step for a critical time step estimate.

To explain how the Lanczos method can effectively be used in an explicit, transient dynamics code, we begin with a simple case study. In this case study, we compute the critical time step using
the Lanczos method at some time step and then assume that this critical time step value remains constant for a subsequent number of time steps, $n_L$. We only call the Lanczos method once during the $n_L$ time steps. (In reality, the critical time step in an explicit, transient dynamics code like Presto changes with each time step. We address this issue of the changing time step when we present the details for using the Lanczos method in a cost-effective manner.) For this case study, we also assume that the computational cost of an element-based estimate for the critical time step is part of the cost of an internal force calculation. The cost of the element-based time step estimate is a small part of the overall internal force calculations. Finally, for our initial discussion, we assume no contact. We address the issue of contact further in the discussion.

Assume that the Lanczos method computes a global estimate for the critical time step of $\Delta t_L$, which is the value to be used for $n_L$ time steps. At the end of the $n_L$ time steps, the analysis time for the code has been incremented by an amount $\Delta T$, which is computed simply as

$$\Delta T = n_L \Delta t_L.$$ (3.2)

If the element-based estimate for the time step is $\Delta t_e$ and the number of time steps required to increment the analysis time by $\Delta T$ is $n_e$, then, for the element-based time step, we have

$$\Delta T = n_e \Delta t_e.$$ (3.3)

Because the Lanczos estimate for the critical time step is larger than the element-based estimate, we know that $n_e > n_L$. Let us define the ratio $r$ as

$$r = \frac{\Delta t_L}{\Delta t_e} = \frac{n_e}{n_L}.$$ (3.4)

The ratio $r$ is greater than 1.

Now that we have determined the relation between the number of steps required for a Lanczos-based critical time step estimate versus the element-based critical time step estimate to achieve the same analysis time increment, let us examine the computational costs for these two cases in terms of CPU time. Designate the CPU cost for a time step as $\Delta t_{IF}$. If the number of Lanczos vectors required to obtain the critical time step estimate is $N_L$, then the total computational cost of the Lanczos method and the $n_L$ time steps is

$$n_L \Delta t_{IF} + N_L \Delta t_{IF}.$$ (3.5)

If we use the element-based method, the total computational cost is

$$n_e \Delta t_{IF}.$$ (3.6)

Recall that we have chosen $n_L$ and $n_e$ so that we have the same analysis time increment $\Delta T$ even though we have different critical time steps. Now, we must determine the point at which the computational cost for the Lanczos-based critical time step calculations is the same as the cost for the element-based critical time step calculations. This is simply the point at which
3.2. OTHER CRITICAL TIME STEP METHODS

\[ n_e \Delta t_{IF} = n_L \Delta t_{IF} + N_L \Delta t_{IF} . \]  (3.7)

If we rearrange the above equation to eliminate \( \Delta t_{IF} \) and make use of the ratio \( r \), then we obtain

\[ n_e = \frac{N_L}{1 - 1/r} . \]  (3.8)

Consider the case of \( r = 1.25 \) and \( N_L = 20 \). When \( n_L = 80 \) and \( n_e = 100 \), the above equations show that the calculations with the Lanczos-based critical time step and the calculations with the element-based time step give the same analysis time for the same computational expense. If we use the Lanczos-based critical time step \( \Delta t_L \) for more than eighty iterations, then the Lanczos-based approach becomes cost effective. Our above equations have established the "break-even" point at which it becomes cost effective to use the Lanczos method to reduce computational costs by overcoming the initial cost of the Lanczos calculations with the larger critical time step.

We can build on what we have done thus far to account for contact. Suppose that the computational cost of contact over a time step is some multiple \( m \) of the computational cost of the internal force calculation \( \Delta t_{IF} \). Then the point at which the computational cost for the Lanczos-based calculations is the same as the computational cost for the element-based calculations is

\[ (1 + m)n_L \Delta t_{IF} + N_L \Delta t_{IF} = (1 + m)n_e \Delta t_{IF} . \]  (3.9)

For the case with contact,

\[ n_e = \frac{N_L}{(1 + m)(1 - 1/r)} . \]  (3.10)

Again, consider the case of \( r = 1.25 \) and \( N_L = 20 \). Assume the computational cost of contact calculations is the same as an internal force calculation \( (m = 1) \). For these values, the break-even point is \( n_L = 40 \) and \( n_e = 50 \). The added computational cost of the contact calculations results in reaching the break-even point with a smaller number of iterations when compared to the case with no contact.

The above derivations let us calculate a break-even point based on our assumptions of a constant critical time step. Considering that a typical analysis will run for tens of thousands of time steps, something on the order of 100 steps represents a reasonable number of steps to recoup the cost of the Lanczos calculations. Whether or not the cost of the Lanczos calculations can be recouped in something on the order of 100 calculations depends heavily upon \( N_L \). If \( N_L \) is sufficiently small, we can recoup the cost of the Lanczos calculations in a reasonable number of steps.

Some computational studies indicate that \( N_L \) is in an acceptable range for many problems. The Lanczos method computes a good estimate for the maximum eigenvalue with a small number of Lanczos vectors, \( N_L \), compared to the number of degrees of freedom in a problem. Some component studies show that, for a problem with between 250,000 and 350,000 degrees of freedom, one can obtain a good estimate for the maximum eigenvalue with only twenty Lanczos vectors. A large-scale study of a model involving 1.7 million nodes (5.1 million degrees of freedom) showed
that only forty-five Lanczos vectors were required to obtain a good estimate of the maximum
eigenvalue. These examples demonstrate that the number of Lanczos vectors required for a good
maximum eigenvalue estimate is very small when compared to the number of degrees of freedom
for a problem. When $N_L$ is in the range of twenty to forty-five, Equations 3.7 and 3.10 show that,
with an increase in the time step on the order of 1.2 to 1.25, we can recoup the cost of the Lanczos
method in a reasonable number of time steps.

Now that we have determined we can recoup the cost of the Lanczos calculations in a reasonable
number of time steps, let us look at the issue of reusing a Lanczos-based estimate in some manner.

3.2.1.2 Controls for Lanczos Method

As indicated in the above discussion, the Lanczos method can be used in a cost-effective manner
in an explicit, transient dynamics code if a Lanczos calculation can be performed and the Lanczos-
based estimate for the critical time step can be reused in some way over a number of subsequent
time steps. This section presents an approach for reusing a Lanczos-based estimate over a number
of time steps so that we maintain a critical time step estimate that is close to the theoretical max-
imum value in between the calls to the Lanczos method. The approach discussed here makes use
of the element-based critical time step estimate at each time step.

We start our approach with a Lanczos calculation to determine the maximum eigenvalue. The
Lanczos method converges to the maximum eigenvalue from below, which means that the method
underestimates the maximum eigenvalue. Because the critical time step depends on the inverse of
the maximum eigenvalue, we overestimate the critical time step. It is necessary, therefore, to scale
back the critical time step estimate from the Lanczos method so that the calculations in the explicit
time-stepping scheme do not become unstable. Our approach for determining a scaled-back value
for the maximum critical time step makes use of the element-based time step estimate. Again, let
$\Delta t_L$ be the critical time step estimate from the Lanczos method and $\Delta t_e$ be the critical time step
estimate from the element-based calculations. The scaled-back estimate for the critical time step,$\Delta t_s$, is computed from the equation

$$\Delta t_s = \Delta t_e + f_s (\Delta t_L - \Delta t_e), \quad (3.11)$$

where $f_s$ is a scale factor. (A reasonable value for $f_s$ ranges from 0.9 to 0.95 for our problems.)
This value of $f_s$ puts $\Delta t_s$ close to and slightly less than a theoretical maximum critical time step.

Once $\Delta t_s$ is determined, the ratio

$$t_r = \Delta t_s / \Delta t_e \quad (3.12)$$

is computed. This ratio is then used to scale subsequent element-based estimates for the critical
time step. If $\Delta t_{e(n)}$ is the $n^{th}$ element-based critical time step after the time step where the Lanczos
calculations are performed, then the $n^{th}$ time step after the Lanczos calculations, $\Delta t_{(n)}$, is simply

$$\Delta t_{(n)} = t_r \Delta t_{e(n)}. \quad (3.13)$$
The ratio $t_r$ is used until the next call to the Lanczos method. The next call to the Lanczos method is controlled by one of two mechanisms. With the first mechanism, the user can set the frequency with which the Lanczos method is called. The user can set a parameter so that the Lanczos method is called only once every $n$ time steps. This number remains fixed throughout an analysis. With the second mechanism, the user can control when the Lanczos method is called based on changes in the element-based critical time step. For this second mechanism, the change in the element-based critical time step estimate is tracked. Suppose the element-based critical time step at the time the Lanczos method was called is $\Delta t_e$. At the $n^{th}$ step after the call to the Lanczos method, the element-based critical time step is $\Delta t_{e(n)}$. If the value

$$\Delta t_{lim} = \frac{|\Delta t_{e(n)} - \Delta t_e|}{\Delta t_e}$$

(3.14)

is greater than some limit set by the user, then the Lanczos method will be called. If there is a small, monotonic change in the element-based critical time step over a large number of time steps, this second mechanism will result in the Lanczos method being called. Or if there is a large, monotonic change in the element-based critical time step over a few time steps, the Lanczos method will also be called.

These two mechanisms for calling the Lanczos method can be used together. For example, suppose the second mechanism (the mechanism based on a change in the element-based time step) results in a call to the Lanczos method. This resets the counter for the first mechanism (the mechanism using a set number of time steps between calls to the Lanczos method).

This approach for reusing a Lanczos-based time step estimate has been implemented in Presto, and it has been used for a number of studies. One of the component studies, as indicated previously, used the same scale factor for $n_L = 1700$ iterations. The break-even point for this problem is $n_e = 45$ time steps (not accounting for contact, which was a part of the component modeling). For this particular problem, the extended use of the Lanczos estimate reduced the computational cost to 56% of what it would have been with the element-based time step.

Not all problems will lend themselves to reusing one Lanczos-based estimate for thousands of time steps. However, if it is possible to use the Lanczos-based estimate for two to three times the number of time steps required to reach the break-even point, we begin to see a noticeable reduction in the total number of time steps required for a problem.

### 3.2.1.3 Scale Factor for Lanczos Method

When the Lanczos method is called for a given time step, it must appear that the calculations are using the constant tangent stiffness matrix $K_T$ for all iterations. As indicated previously, we use the internal force calculations to generate the product $K_T p_j$ (for the $j^{th}$ iteration) in the Lanczos calculations. Any vector $p_j$, as calculated by the Lanczos method, may be such that it represents large-strain behavior and moves the internal force calculations into a nonlinear regime. It is necessary to scale the $p_j$ vectors so that the internal force calculations are in a small-strain regime, which makes it appear that we are working with a constant tangent stiffness matrix. The vectors $p_j$ must be scaled so that they represent velocities associated with small strain. When properly scaled
vectors are sent to the internal force calculation, the internal force calculation effectively becomes a matrix \( \times \) vector product with a constant tangent stiffness matrix for all iterations during a given call to the Lanczos method.

The scale factor for the \( \mathbf{p}_j \) vectors, which we will designate as \( v_{sf} \), must not be too small, as this will create round-off problems and give a bad estimate for the critical time step. If the scale factor is too large, we violate the above restriction of a constant tangent stiffness matrix.

There are two approaches for controlling the scale factor when the Lanczos method is used to compute the maximum eigenvalue. These approaches are discussed in Section 3.2.1.5.

### 3.2.1.4 Accuracy of Eigenvalue Estimate

Every time a new Lanczos vector is computed, we obtain an additional eigenvalue for our model and, in general, a better estimate for the maximum eigenvalue (and hence a better estimate for the critical time step). The Lanczos method can compute a good value for the maximum eigenvalue with a very small number of total computed eigenvalues compared to the number of degrees of freedom in a problem. There are examples, as previously indicated, of problems with 250,000 to 350,000 degrees of freedom where we have obtained a good estimate of the critical time step with twenty eigenvalues. In one problem with 5.1 million degrees of freedom, we obtained a good estimate of the critical time step with forty-five eigenvalues.

A user could, in theory, determine a reasonable number of eigenvalues necessary for obtaining a good estimate of the maximum eigenvalue based on the above information on model size and the number of eigenvalues required for a good maximum eigenvalue estimate. The user could test the validity of the choice of the number of eigenvalues by increasing the number of eigenvalues slightly and comparing the maximum eigenvalue estimate obtained with the larger number of eigenvalues to the original maximum eigenvalue estimate obtained with the smaller number of eigenvalues. If the change in the two maximum eigenvalue estimates (larger versus smaller total number of eigenvalues) is small, then the original estimate for the number of eigenvalues is reasonably accurate.

As an alternative to directly specifying the number of eigenvalues to be computed, a convergence tolerance could be set on the change in the magnitude of the maximum eigenvalue as additional eigenvalues (Lanczos vectors) are computed. Let \( \theta_{\text{max}, \ n} \) be the maximum eigenvalue calculated corresponding to \( n \) eigenvalues (Lanczos vectors), and let \( \theta_{\text{max}, \ n+1} \) be the maximum eigenvalue corresponding to \( n + 1 \) eigenvalues (Lanczos vectors). The eigenvalues would be computed until

\[
\frac{|\theta_{\text{max}, \ n+1} - \theta_{\text{max}, \ n}|}{\theta_{\text{max}, \ n+1}} \leq \text{tol}
\]

is less than some tolerance. (We will now refer to the value of Equation (3.15) as the convergence measure.) If we calculate the convergence measure for a sequence of maximum eigenvalues computed by the Lanczos method, we will not necessarily see a monotonic decrease in the convergence measure for all time. Typically, the convergence measure will initially show a monotonically decreasing value for an increasing \( n \), and then the convergence measure will show a monotonically increasing value for an increasing \( n \). (The phase in which the convergence measure increases is usually very small, on the order of one to two iterations.) After the phase in which the convergence
measure monotonically increases, there is then a phase in which the convergence measure begins a
long (over many iterations) monotonic decrease. This behavior (decrease of the convergence mea-
ure, slight increase, then long monotonic decrease) is typical of Krylov methods, of which the
Lanczos method is one. Using the convergence measure to determine the number of eigenvalues
to be computed for a problem is a reasonable option, but some care must be taken in setting the
tolerance for the convergence measure.

Both of the techniques just discussed are offered as a way to set the maximum number of eigenval-
ues required to obtain an accurate eigenvalue estimate for a model. These techniques are discussed
further in Section 3.2.1.5.

3.2.1.5 Lanczos Parameters Command Block

BEGIN LANCZOS PARAMETERS <string>lanczos_name
   STARTING VECTOR = <string>STRETCH_X|STRETCH_Y|STRETCH_Z|
                     ISOTHERMAL(ISOTHERMAL)
   INCREASE OVER STEPS = <integer>incr_int(5)
   NUMBER EIGENVALUES = <integer>num_eig(150)
   EIGENVALUE CONVERGENCE TOLERANCE = <real>converge_tol(0.5e-3)
   SMALL STRAIN = <real>small_strain(1.0e-3)
   VECTOR SCALE = <real>vec_scale(1.0e-5)
   SCALE FACTOR = <real>time_scale(0.9)
   UPDATE ON TIME STEP CHANGE = <real>tstep_change(0.10)
   UPDATE STEP INTERVAL = <integer>step_int(500)
END [LANCZOS PARAMETERS <string>lanczos_name]

If you use the Lanczos method to compute a critical time step, there should be only one LANCZOS
PARAMETERS command block, and it should appear in the region. If you have a LANCZOS
PARAMETERS command block, you should not specify a NODE BASED TIME STEP PARAMETERS or a POWER
METHODS PARAMETERS command block. If you use the Lanczos method to compute the criti-
cal time step, the time step increase factor (default or user-specified) will be used to control the
increase in the time step estimate; the time step scale factor (default or user-specified) will not
be used. These factors are specified in the PARAMETERS FOR PRESTO REGION portion of a
TIME STEPPING BLOCK in the TIME CONTROL command block.

The Lanczos method requires some type of starting vector. This is determined by the STARTING
VECTo command line. The various options available for this command line will generate a dis-
placement vector that stretches your model in the x-, y-, or z-direction, or in all three directions
(x, y, and z) at once. (STRETCH_X stretches the model in the x-direction, STRETCH_Y stretches
the model in the y-direction, STRETCH_Z stretches the model in the z-direction, and ISOTHERMAL
stretches the model in all three directions at once.) The displacement vector then serves as a basis
for generating the starting vector \( r_0 \) in the initialization phase of the Lanczos method. The Lanczos
method appears to be fairly insensitive to the choice of a starting vector. The default starting vector
is the ISOTHERMAL option. You may encounter cases where the use of one of the other options for
a starting vector—STRETCH_X, STRETCH_Y, or STRETCH_Z—may result in a slight increase in
accuracy for the critical time step estimate for a given number of eigenvalues. These other options
(STRETCH_X, STRETCH_Y, and STRETCH_Z) are offered for these special cases.

The INCREASE OVER STEPS command line determines how many steps, i.e., incr_int, are used to transition from an element-based critical time step estimate to the Lanczos-based estimate at the beginning of an analysis. The user may want to increase from the element-based estimate to the Lanczos-based estimate over a number of time steps if the difference between these two estimates is large. The value of incr_int for this command line defaults to 5.

As indicated in Section 3.2.1.4, some number of eigenvalues must be computed by the Lanczos method to obtain a good estimate for the maximum eigenvalue for a given finite element model. As one option, the user can simply specify the number of eigenvalues to be computed by the Lanczos method by using the NUMBER EIGENVALUES command line. The default value for num_eig in this command line is 150. As an alternative, the user can specify a tolerance on the convergence measure defined in Equation (3.15). The tolerance is set with the EIGENVALUE CONVERGENCE TOLERANCE command line. The default value for the convergence tolerance, converge_tol, is 0.5 x 10^{-3}. (This default value may change in the future as we gain more experience with the Lanczos method.)

By default, the convergence measure (with the default value of 0.5 x 10^{-3}) is used to determine the number of eigenvalues to be computed. If neither the EIGENVALUE CONVERGENCE TOLERANCE command line nor the NUMBER EIGENVALUES command line appears in the LANCZOS PARAMETERS command block, then the convergence measure will be used to determine the number of eigenvalues. If the EIGENVALUE CONVERGENCE TOLERANCE command line appears in the command block with a specified tolerance other than the default value, then the number of eigenvalues computed will be determined by the convergence measure and the user-specified tolerance. If the NUMBER EIGENVALUES command line appears in the LANCZOS PARAMETERS command block, then the user-defined number of eigenvalues will be used to set the number of eigenvalues computed by the Lanczos method.

The recommended technique for determining the number of eigenvalues is to use the convergence measure option with the default tolerance. If you use this technique, neither the NUMBER EIGENVALUES command line nor the EIGENVALUE CONVERGENCE TOLERANCE command line should be included in the LANCZOS PARAMETERS command block.

As indicated in Section 3.2.1.3, it is necessary to scale one of the vectors (with a scale factor v_s_f) in the Lanczos calculations so that it appears we are always working with a constant tangent stiffness each time we call the Lanczos method. There are two approaches for determining the scale factor. With the first approach, the user can specify the value of a small strain for a particular model by using the SMALL STRAIN command line. (As long as the internal force calculation inside the Lanczos method is working with a vector that approximates small-strain behavior, it will appear that we are working with a constant tangent stiffness inside the Lanczos method.) The value for v_s_f is then computed based on your specification for what constitutes a small strain in the model. (The default value for small_strain is 1.0 x 10^{-3}.) With the second approach for determining the scale factor, the user can specify a value for v_s_f directly by using the VECTOR SCALE command line. The default value for v_s_f, the vec_scale parameter in that command line, is 1.0 x 10^{-5}. A number of tests have established that this value for the scale factor, 1.0 x 10^{-5}, works well for a range of models encountered at Sandia National Laboratories. If the user wants to use the option of directly specifying the scale factor, it is possible to determine whether a particular scale factor
3.2. OTHER CRITICAL TIME STEP METHODS

is suitable for a particular problem. Take a scale factor $v_s$, plus values on either side of it, say, $0.9 \times v_s$ and $1.1 \times v_s$. If all three of these scale factor values produce almost the same estimate for the critical time step for a particular model, then the value for $v_s$ meets the criterion for an acceptable scale factor.

By default, the small-strain approach (with the default value of $1.0 \times 10^{-3}$) is used to determine a scale factor. If neither the SMALL STRAIN command line nor the VECTOR SCALE command line appears in the LANCZOS PARAMETERS command block, then the small-strain value will be used to calculate the scale factor. If the SMALL STRAIN command line appears in the command block with any value other than the default value and the VECTOR SCALE command line does not appear in the command block, then the vector scale will be determined by the user-specified value for the small strain. If the VECTOR SCALE command line does appear in the LANCZOS PARAMETERS command block, then the vector scale will be determined by the user-specified value for the vector scale.

The recommended way of determining the scale factor is to use the small-strain approach with the default small-strain value. If you follow this advice, neither the SMALL STRAIN command line nor the VECTOR SCALE command line should be included in the LANCZOS PARAMETERS command block.

As indicated previously, the scale factor must not be too small, as this will create round-off problems and give a bad estimate for the critical time step. If the scale factor is too large, we violate the above restriction of a constant tangent stiffness matrix.

The SCALE FACTOR command line sets the factor $f_s$ in Equation (3.11). The value for $f_s$, i.e., time_scale, is set to 0.9. More experience with the Lanczos method will help us determine whether a slightly larger value of $f_s$ can be used as a default.

The UPDATE ON TIME STEP CHANGE command line sets the value for $\Delta t_{lim}$ in Equation (3.14). If the change in the element-based critical time step estimate as given by Equation (3.14) exceeds the value for $\Delta t_{lim}$, then the Lanczos method is called for a new estimate for the critical time step. The default value for $\Delta t_{lim}$, i.e., tstep_change, is 0.10.

The UPDATE STEP INTERVAL command line sets the number of step intervals at which the Lanczos method is called. If step_int is set to 1000, the Lanczos method will be called every one thousand steps to compute an estimate for the critical time step. (The default value of step_int is 500.) This control mechanism interacts with the control established by the UPDATE ON TIME STEP CHANGE command line. Suppose we have set step_int to 1000, and we have computed 800 steps since the last call to the Lanczos method. If $\Delta t_{lim}$ has been set to 0.15 and we exceed this value at step 800, then the change in the element-based time step will result in the Lanczos method being called. The counter for keeping track of the number of step intervals since the last Lanczos computation will be reset to zero. The next call to the Lanczos method will occur again in one thousand steps, unless we again exceed the change in the element-based time step.
3.2.2 Power Method

The power method is a simple iterative technique that gives an estimate for the maximum eigenvalue. Consider the following form of the eigenvalue problem, which is useful for our explicit transient dynamics problem.

\[
\mathbf{K}_T \mathbf{x}_i - \theta_i \mathbf{M} \mathbf{x}_i = 0 \quad (3.16)
\]

Reformulate the problem as

\[
[\mathbf{M}]^{-1} \mathbf{K}_T \mathbf{x}_i - \theta_i \mathbf{x}_i = 0 .
\]

Denote the matrix product \([\mathbf{M}]^{-1} \mathbf{K}_T\) as the matrix operator \(\mathbf{A}\). The eigenvalue problem is now

\[
\mathbf{A} \mathbf{x}_i - \theta_i \mathbf{x}_i = 0 .
\]

The maximum eigenvalue for the problem in Equation (3.18) can be computed with the following iterative process:

\[
\text{for } i = 1, n
\]
\[
\mathbf{x}_i = \mathbf{Ax}_{i-1}
\]
\[
\mathbf{x}_i = \mathbf{x}_i / \| \mathbf{x}_i \|
\]
\[
\theta_i = [\mathbf{x}_i]^T \mathbf{Ax}_i
\]
\[
\text{end}
\]

The value \(\theta_i\) is the \(i^{th}\) estimate for the maximum eigenvalue. As \(n\) increases, the power method should yield a more accurate estimate for the maximum eigenvalue. So, just as with the Lanczos method, the power method must iterate at some given time step to obtain an estimate for the maximum eigenvalue at that time step. The details for the above form of the power method are described in Reference 2.

Like the Lanczos method, the power method requires the use of an internal force calculation. The power method, however, is somewhat simpler than the Lanczos method. The power method requires that one vector and one scalar be computed. The Lanczos method requires the computation of five vectors and two scalars. Further, the power method yields a direct estimate for the maximum eigenvalue, whereas the Lanczos method requires that the maximum eigenvalue be extracted from a tridiagonal matrix.

If the sequence of eigenvalues for an analysis problem is

\[
| \lambda_1 | > | \lambda_2 | \geq \cdots \geq | \lambda_n | ,
\]

then the rate of convergence to the maximum eigenvalue depends on the ratio

\[
\frac{| \lambda_1 |}{| \lambda_2 |} .
\]

Depending on the magnitudes of \(| \lambda_1 |\) and \(| \lambda_2 |\), the rate of convergence could be rather slow. The power method, for a given problem, may not converge to as accurate an estimate for the maximum eigenvalue as quickly as the Lanczos method. We should be careful, however, in how
we interpret this convergence property for the power method. For many of our problems, we probably have a large number of eigenvalues clustered just below the maximum eigenvalue. The power method may give a reasonable estimate for the maximum eigenvalue in a relatively small number of iterations. The power method may converge quickly to some eigenvalue estimate that is just below the maximum eigenvalue. Convergence to the maximum eigenvalue, in terms of accuracy to many digits, might then be very slow. However, one would still have an adequate estimate for the maximum eigenvalue to set a value for the critical time step.

One of the advantages of the power method is that we can use the last value for $x_i$ from a previous call to the power method as a starting vector for our current call to the power method and converge quickly (for some problems) to an accurate estimate for the maximum eigenvalue. Consider the following scenario. We make an initial call to the power method using some arbitrary $x_0$ starting vector. We obtain a good estimate for the maximum eigenvalue after $n$ iterations. After some number of time steps, we again call the power method and we use $x_n$ from the previous call to the power method as our current starting vector. Because we are solving nonlinear problems, the matrix operator, $A$, has most likely changed from the time when we made the initial call to the power method. If the changes in the matrix operator are small, then $x_n$ should be an excellent choice for the starting vector, and we should converge quickly to a good estimate for the maximum eigenvalue. This behavior, quick convergence to a good eigenvalue estimate using a prior value of $x_n$ as a starting vector, has been observed in some sample problems. We discuss this issue of restarting the power method using a previous $x_n$ in more detail in Section 3.2.2.1.

Obtaining a cost-effective and user-friendly implementation of the power method requires addressing the same issues discussed above for an automated implementation of the Lanczos method. First, we must determine some scheme to call the power method on an intermittent basis so that it is cost effective. The control mechanism for calling the Lanczos method on an intermittent basis can also be used for the power method. Second, the $x$ vector must be scaled appropriately before it is used in the internal force calculations. (For the Lanczos method, we must scale the vector $p$.) Finally, we need to terminate the power method. A tolerance on the value in Equation (3.15) can be set to terminate the method. (Setting a tolerance on Equation (3.15) is the same approach used for the Lanczos method.)

### 3.2.2.1 Power Method with Constant Time Steps

The cost of making one iteration for the power method is approximately the cost of an internal force calculation. As indicated previously, the cost of one iteration for the Lanczos method (the calculation of a Lanczos vector) is also approximately the cost of an internal force calculation. Therefore, the equations developed in Section 3.2.1.1 are also applicable for determining when the power method can be used in a cost-effective manner. Recall that the equation

$$n_e = \frac{N_L}{1 - 1/r}$$  \hspace{1cm} (3.21)

in Section 3.2.1.1 gives the number of time steps for the break-even point at which it becomes cost effective for the case of no contact to use the Lanczos method to reduce computational costs by overcoming the initial cost of the Lanczos calculations with the larger critical time step. In the
above equation, \( N_L \) is the number of Lanczos iterations, and \( r \) is the ratio of the Lanczos-based critical time to the element-based time step estimate. This equation is directly applicable to the power method because the cost of one iteration in the power method is similar to the cost of one iteration in the Lanczos method. (The variable \( N_L \) becomes the number of iterations for the power method.)

Now let us return to the scenario in Section 3.2.2 where we look at restarting the power method with the last value for \( x_i \) from a previous call to the power method. We make an initial call to the power method using some arbitrary \( x_0 \) starting vector. We obtain a good estimate for the maximum eigenvalue after \( n \) iterations. Our estimate for the critical time step based on the maximum eigenvalue gives us a value of 1.25 for \( r \). After some number of time steps, we again call the power method, and we use \( x_n \) from the previous call to the power method as our current starting vector. In our second call to the power method, the power method converges to a good estimate for the maximum eigenvalue in two iterations. The break-even point where we recoup the cost of the power method (in our second call) is ten time steps. If the power method converges to a good estimate for the maximum eigenvalue in three iterations, then the break-even point where we recoup the cost of the power method (in our second call) is fifteen time steps. There are some problems where we can obtain a good estimate for the maximum eigenvalue in two or three iterations when we use the last value for \( x_n \) from a previous call to the power method as our starting vector for the current call to the power method. For the case where we can converge to a good estimate for the maximum eigenvalue in two or three iterations, we can easily call the power method once every forty or fifty time steps and use the power method to improve the time step estimate in a cost-effective manner. Over a time span of forty or fifty time steps, matrix operator \( A \), as defined in Equation (3.18) may change by only a small amount for a large class of problems. If matrix operator \( A \) changes by a small amount, then using the last value of \( x_n \) from a previous call to the power method provides an excellent starting vector and gives us quick convergence. This ability of the power method to converge quickly by using previous information makes it a viable scheme for calculating the maximum eigenvalue and producing a critical time step estimate.

For a problem with contact, the equations derived for the Lanczos method (with contact) in Section 3.2.1.1 are also applicable to the power method. For the power method, as in the case of the Lanczos method, the added computational cost of the contact calculations results in reaching a break-even point with a smaller number of iterations when compared to a case where there is no contact.

### 3.2.2.2 Controls for Power Method

Using the power method is similar to using the Lanczos method in that we must be able to perform a power method calculation and reuse the power method estimate for the critical time step in some way over a number of subsequent time steps. The approach for reusing a power method estimate for the critical time step over a number of time steps is the same as the approach for reusing a Lanczos-based estimate over a number of time steps as described in Section 3.2.1.2. The approach discussed in Section 3.2.1.2 presents a way to reuse a maximum eigenvalue time step estimate over a number of time steps so that we maintain a critical time step estimate that is close to the theoretical maximum value in between the calls to the maximum eigenvalue calculations. The
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approach discussed in in Section 3.2.1.2 makes use of the element-based critical time step estimate at each time step.

3.2.2.3 Scale Factor for Power Method

When the power method is called for a given time step, it must appear that the calculations are using a constant matrix operator, $A$, for all iterations. The $A$ operator is the product of the inverse of the mass matrix $M^{-1}$ and the tangent stiffness matrix $K_T$ for the problem. The mass matrix is a constant. Therefore, we must assure that we are working with what is effectively a constant tangent stiffness matrix for all iterations during a call to the power method. This is the same requirement that we encounter in the Lanczos method (see Section 3.2.1.3). For the power method, we use the internal force calculations to generate the product $Ax$ by first computing the internal forces using $x$, which gives us the product $K_T x$, and then multiplying the internal force results by the inverse of the mass matrix. Any vector $x$, as calculated by the power method, may be such that it represents large-strain behavior and moves the internal force calculations into a nonlinear regime. It is necessary to scale the $x$ vectors so that the internal force calculations are in a small-strain regime, which makes it appear that we are working with a constant tangent stiffness matrix. The vectors $x$ must be scaled so that they represent velocities associated with small-strain calculations. When properly scaled vectors are sent to the internal force calculation, the internal force calculation becomes a matrix $\times$ vector product with a constant tangent stiffness matrix for all iterations during a given call to the power method.

The scale factor for the $x$ vectors, which we will designate as $v_{xf}$, must not be too small, as this will create round-off problems and give a bad estimate for the critical time step. If the scale factor is too large, we violate the above restriction of a constant tangent stiffness matrix.

There are two approaches for controlling the scale factor when the power method is used to compute the maximum eigenvalue. These approaches are discussed in Section 3.2.2.5.

3.2.2.4 Accuracy of Eigenvalue Estimate

To use the power method efficiently, it is best not to specify a set number of iterations for every instance when the power method is called. Instead, some tolerance should be set on the convergence measure defined in Equation (3.15). The initial call to the power method may take a significant number of iterations to produce a good estimate for the maximum eigenvalue. On subsequent calls to the power method, the number of iterations to converge to a good estimate for the maximum eigenvalue should be quite small when we use previous values of $x$ as a starting vector.

For the power method, we rely on the convergence measure defined by Equation (3.15) to control the number of iterations. The user can set an upper limit on the number of iterations for the power method. Control of the number of iterations for the power method is discussed in more detail in Section 3.2.2.5.
3.2.2.5 Power Method Parameters Command Block

BEGIN POWER METHOD PARAMETERS <string>powermethod_name
STARTING VECTOR = <string>STRETCH_X|STRETCH_Y|STRETCH_Z|
                   ISOTHERMAL(ISOTHERMAL)
INCREASE OVER STEPS = <integer>incr_int(5)
NUMBER ITERATIONS = <integer>num_iter(150)
EIGENVALUE CONVERGENCE TOLERANCE =
                   <real>converge_tol(0.5e-3)
SMALL STRAIN = <real>small_strain(1.0e-3)
VECTOR SCALE = <real>vec_scale(1.0e-5)
SCALE FACTOR = <real>time_scale(0.9)
UPDATE ON TIME STEP CHANGE = <real>tstep_change(0.10)
UPDATE STEP INTERVAL = <integer>step_int(50)
END [POWER METHOD PARAMETERS <string>powermethod_name]

If you use the power method to compute a critical time step, there should be only one POWER
METHOD PARAMETERS command block, and it should appear in the region. If you have a
POWER METHOD PARAMETERS command block, you should not specify a command block for the node-
based method or the Lanczos method. If you use the power method to compute the critical time
step, the time step increase factor (default or user-specified) set in the TIME CONTROL command
block will be used to control the increase in the time step estimate; the time step scale factor (default
or user-specified) set in the TIME CONTROL command block will not be used. These factors are
specified in the PARAMETERS FOR PRESTO REGION portion of a TIME STEPPING BLOCK in
the TIME CONTROL command block.

The power method requires some type of starting vector. This is determined by the STARTING
VECTOR command line. The various options available in this command line will generate a dis-
placement vector that stretches your model in the x-, y-, or z-direction, or in all three directions
(x, y, and z) at once. (STRETCH_X stretches the model in the x-direction, STRETCH_Y stretches
the model in the y-direction, STRETCH_Z stretches the model in the z-direction, and ISOTHERMAL
stretches the model in all three directions at once.) The displacement vector then serves as a basis
for generating the starting vector \( x_0 \) in the initialization phase of the Lanczos method. The default
starting vector is the ISOTHERMAL option. You may encounter cases where use of one of the other
options for a starting vector—STRETCH_X, STRETCH_Y, or STRETCH_Z—may result in a slight
increase in accuracy for the critical time step estimate for a given number of iterations. These
other options (STRETCH_X, STRETCH_Y, and STRETCH_Z) are offered for these special cases.

The INCREASE OVER STEPS command line determines how many steps, incr_int, are used to
transition from an element-based critical time step estimate to the power method estimate at the
beginning of an analysis. The user may want to increase from the element-based estimate to the
power method estimate over a number of time steps if the difference between these two estimates
is large. The value of incr_int defaults to 5.

As indicated in Section 3.2.2.4, some number of iterations are required by the power method to
obtain a good estimate for the maximum eigenvalue for a given model. The number of iterations is
controlled by the tolerance set for the convergence measure given in Equation (3.15). The tolerance
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is set with the `EIGENVALUE CONVERGENCE TOLERANCE` command line. The default value for the convergence tolerance, `converge_tol` is $0.5 \times 10^{-3}$. (This default value may change in the future as we gain more experience with the power method.)

The user can set an upper limit on the number of iterations for the power method by using the `NUMBER ITERATIONS` command line. If the number of iterations in the power method exceeds the value set by `num_iter`, then the power method is terminated. Otherwise, the iterative process in the power method is terminated by the tolerance set on the convergence measure. The default value for `num_iter` is 150.

As indicated in Section 3.2.2.3, it is necessary to scale the vectors $x_i$ (with a scale factor $v_{sf}$) in the power method calculations so that it appears we are always working with a constant tangent stiffness each time we call the power method. There are two approaches for determining the scale factor. With the first approach, the user can specify the value of a small strain for a particular model by using the `SMALL STRAIN` command line. (As long as the internal force calculation inside the power method is working with a vector that approximates small-strain behavior, it will appear that we are working with a constant tangent stiffness inside the power method.) The value for $v_{sf}$ is then computed based on your specification for what constitutes a small strain in the model. (The default value for `small_strain` is $1.0 \times 10^{-3}$.) With the second approach for determining the scale factor, the user can specify a value for $v_{sf}$ directly by using the `VECTOR SCALE` command line. The default value for $v_{sf}$, the `vec_scale` parameter in that command line, is $1.0 \times 10^{-5}$. A number of tests have established that this value for the scale factor, $1.0 \times 10^{-5}$, works well for a range of models encountered at Sandia National Laboratories. If the user wants to use the option of directly specifying the scale factor, it is possible to determine whether a particular scale factor is suitable for a particular problem. Take a scale factor $v_{sf}$, plus values on either side of it, say, $0.9 \times v_{sf}$ and $1.1 \times v_{sf}$. If all three of these scale factor values produce almost the same estimate for the critical time step for a particular model, then the value for $v_{sf}$ meets the criterion for an acceptable scale factor.

By default, the small-strain approach (with the default value of $1.0 \times 10^{-3}$) is used to determine a scale factor. If neither the `SMALL STRAIN` command line nor the `VECTOR SCALE` command line appears in the `POWER METHOD PARAMETERS` command block, then the default small-strain value will be used to calculate the scale factor. If the `SMALL STRAIN` command appears in the command block with any value other than the default value and the `VECTOR SCALE` command line does not appear in the command block, then the vector scale will be determined by the user-specified value for the small strain. If the `VECTOR SCALE` command line does appear in the `POWER METHOD PARAMETERS` command block, then the vector scale will be determined by the user-specified value for the vector scale.

The recommended way of determining the scale factor is to use the small-strain approach with the default small-strain value. Thus, if you follow this advice, neither the `SMALL STRAIN` command line nor the `VECTOR SCALE` command line should be included in the `POWER METHOD PARAMETERS` command block.

As indicated previously, the scale factor must not be too small, as this will create round-off problems and give a bad estimate for the critical time step. If the scale factor is too large, we violate the above restriction of a constant tangent stiffness matrix.
The SCALE FACTOR command line sets the factor \( f_s \) in Equation (3.11). The value for \( f_s \), i.e., time_scale, is set to 0.9. More experience with the power method will help us determine whether a slightly larger value of \( f_s \) can be used as a default.

The UPDATE ON TIME STEP CHANGE command line sets the value for \( \Delta t_{lim} \) in Equation (3.14). If the change in the element-based critical time step estimate as given by Equation (3.14) exceeds the value for \( \Delta t_{lim} \), then the power method is called for a new estimate for the critical time step. The default value for \( \Delta t_{lim} \), i.e., tstep_change, is 0.10.

The UPDATE STEP INTERVAL command line sets the number of step intervals at which the power method is called. If step_int is set to 40, the power method will be called every forty steps to compute an estimate for the critical time step. (The default value of step_int is 50.) This control mechanism interacts with the control established by the UPDATE ON TIME STEP CHANGE command line. Suppose we have set step_int to 40, and we have computed thirty-five steps since the last call to the power method. If \( \Delta t_{lim} \) has been set to 0.15 and we exceed this value at step 35, then the change in the element-based time step will result in the power method being called. The counter for keeping track of the number of step intervals since the last power method computation will be reset to zero. The next call to the power method will then occur again in forty steps, unless we again exceed the change in the element-based time step.

### 3.2.3 Node-Based Method

Now that we have developed schemes to make the Lanczos method and power method cost-effective tools for estimation of the critical time step, let us examine the node-based scheme.

The node-based method in Presto will give an estimate for the critical time step that is greater than or equal to the element-based estimate. It may or may not give an estimate for the time step that is close to the maximum value associated with the maximum eigenvalue for the problem. In general, we assume the node-based method will give us an estimate larger than the element-based estimate, but not significantly larger.

If the node-based scheme is used to determine the critical time step for a block of uniform elements (all the same material), then the estimate from the node-based method will be the same as that for the element-based estimate. The node-based estimate begins to diverge from (become larger than) the element-based estimate as the differences in aspect ratios of the elements attached to a node become larger. We can assume, therefore, that if the stiffest part of our structure has a relatively uniform mesh, the node-based method will not give a significantly larger estimate than the element-based method.

The node-based method costs only a fraction of an internal force calculation. However, the node-based method makes use of element time step estimates. Therefore, in order to do the node-based method, one must also do the element-based method. The cost of the node-based method is in addition to the element-based method. The modest increase in the critical step estimate from the node-based method is unlikely to offset the added cost of the node-based method.

To make the node-based method cost-effective, we can use the same methodology that is employed for the Lanczos method. Let \( t_b \) be the estimate for the critical time step from the node-based
method. We define the ratio of the node-based estimate to the element-based estimate as

\[ t_r = \frac{\Delta t_b}{\Delta t_e}. \] (3.22)

This ratio is then used to scale subsequent element-based estimates for the critical time step. If \( \Delta t_{e(n)} \) is the \( n^{th} \) element-based critical time step after the time step where the node-based calculations are performed, then the \( n^{th} \) time step after the node-based calculations, \( \Delta t_{(n)} \), is simply

\[ \Delta t_{(n)} = t_r \Delta t_{e(n)}. \] (3.23)

The ratio \( t_r \) is used until the next call to the node-based method. The next call to the node-based method is controlled by one of two mechanisms described in the Lanczos discussion. The node-based method is called after a set number of times or a significant change in the element-based estimate for the critical time step.

### 3.2.3.1 Node-Based Parameters Command Block

```
BEGIN NODE BASED TIME STEP PARAMETERS <string>nbased_name
  INCREMENT INTERVAL = <integer>incr_int(5)
  STEP INTERVAL = <integer>step_int(500)
  TIME STEP LIMIT = <real>step_lim(0.10)
END [NODE BASED TIME STEP PARAMETERS <string>nbased_name]
```

If you use the node-based method to compute a critical time step, there should be only one NODE BASED TIME STEP PARAMETERS command block, and it should appear in the region. If you use the node-based method to compute the critical time step, you should set the time step scale factor to 1.0 and the time step increase factor to a large number (5.0 is an acceptable value for the time step increase factor). These factors are specified in the PARAMETERS FOR PRESTO REGION portion of a TIME STEPPING BLOCK in the TIME CONTROL command block. If you have a NODE BASED TIME STEP PARAMETERS command block, you should not specify a LANCZOS PARAMETERS command block.

The INCREMENT INTERVAL command line determines how many steps, \( \text{incr\_int} \), are used to transition from an element-based critical time step estimate to the node-based estimate at the beginning of an analysis. The user may want to increase from the element-based estimate to the node-based estimate over a number of time steps if the difference between these two estimates is large. The value of \( \text{incr\_int} \) defaults to 5.

The STEP INTERVAL command line sets the number of step intervals at which the node-based method is called. If \( \text{step\_int} \) is set to 1000, the node-based method will be called every one thousand steps to compute an estimate for the critical time step. (The default value of \( \text{step\_int} \) is 500.) This control mechanism interacts with the control established by the TIME STEP LIMIT command line. Suppose we have set \( \text{step\_int} \) to 1000, and we have computed 800 steps since the last call to the node-based method. If \( \Delta t_{lim} \) has been set to 0.15 and we exceed this value at step
800, then the change in the element-based time step will result in the node-based method being called. The counter for keeping track of the number of step intervals since the last node-based computation will be reset to zero. The next call to the node-based method will occur again in one thousand steps, unless we again exceed the change in the element-based time step.

The `TIME STEP LIMIT` command line sets the value for $\Delta t_{lim}$ in Equation (3.14). If the change in the element-based critical time step estimate as given by Equation (3.14) exceeds the value for $\Delta t_{lim}$, then the node-based method is called for a new estimate for the critical time step. The default value for $\Delta t_{lim}$, i.e., `step_lim`, is 0.10.

## 3.3 Mass Scaling

### 3.3.1 What is Mass Scaling?

Mass scaling allows for arbitrarily increasing the mass of certain nodes in order to increase the global estimate for the critical time step. The nodes where the mass is increased must be associated with those elements that have the minimum time step. By increasing the mass at any node for an element, we have effectively raised the critical time step estimate for that element.

Note that mass scaling does not adjust the value for the density used in the element calculations. Mass scaling only adjusts the mass at the nodes. The net effect of the mass scaling makes it appear, however, as if we have modified the density of selected elements (even though no adjustment has been made to element densities).

**Warning:** Use of mass scaling will introduce error into your analysis. The amount of error incurred is unbounded and can be unpredictable. It is entirely up to the analyst to decide whether mass scaling can be used in a way that does not distort the results of interest.

Mass scaling can be useful in a number of circumstances, as listed below. However, in all of these circumstances, error will be introduced into the calculations. The user must be extremely careful not to introduce excessive error.

- **Quasi-static or rigid-body motion:** If the model or part of a model is undergoing what is basically quasi-static or rigid-body motion, then adding mass may have little effect on the end result.

- **Disparate sizes in element geometry:** A model may contain elements for some portion of the model that are much smaller than the majority of elements in the rest of the model. For example, a model might include screws or gears that are modeled in detail. The elements for the screw threads or gear teeth could be much smaller than elements in other portions of the model. If the dynamics of these parts modeled with small elements (compared to the rest of the mesh) are relatively unimportant, adding mass to them might not affect the quantities of interest.
3.3. MASS SCALING

- Increasing time step for “unimportant” sections of the mesh: For some problems, you may not want part of the mesh to control the time step. Consider a car-crash problem in which the bumper is the first part to strike an object. The crumpling of the bumper could greatly reduce the time step in some elements of the bumper, and these elements would control the time step for the problem. At a later time in the analysis, the effect of the bumper on the overall crash dynamics may not be significant. Mass scaling could be applied to ensure that this now noncritical part (the bumper) is no longer controlling the global time step.

3.3.2 Mass Scaling Command Block

BEGIN MASS SCALING
  # {node set commands}
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list> nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  TARGET TIME STEP = <real>target_time_step
  ALLOWABLE MASS INCREASE RATIO = <real>mass_increase_ratio
  #
  # additional command
  ACTIVE PERIODS = <string list>periods
END MASS SCALING

The MASS SCALING command block controls mass scaling for a specified set of nodes. This command block contains one or more command lines to specify the node set. It also contains two command lines that determine how the actual mass scaling will be applied to the nodes in the node set. In addition to the command lines in the two command groups, there is an additional command line: ACTIVE PERIODS. The ACTIVE PERIODS command line is used to activate or deactivate the mass scaling for certain time periods.

Multiple MASS SCALING command blocks can exist to apply different criteria to different portions of the mesh at different times. For any given set of MASS SCALING command blocks, mass will only be added to a node if doing so will allow increasing the global time step. The amount of artificial mass added to a node will vary in time as the mesh deforms and moves. The added mass computation is redone every time the nodal-based time step estimate is recomputed.

NOTE: Mass scaling must be used in conjunction with the node-based time step estimation method. Consult with the preceding sections for a description of the node-based method for estimating the critical time step.

Following are descriptions of the different command groups and the ACTIVE PERIODS command line.
CHAPTER 3. TIME STEP CONTROL IN PRESTO

3.3.3 Node Set Commands

The \{node set commands\} portion of the MASS SCALING command block specifies the nodes associated with the boundary condition. This portion of the command block can include some combination of the following lines:

\begin{verbatim}
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list> nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
\end{verbatim}

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes for mass scaling. There must be at least one NODE SET, SURFACE, BLOCK, or INCLUDE ALL BLOCKS command line in the command block.

3.3.3.1 Mass Scaling Commands

The MASS SCALING command block may contain either a

\texttt{TARGET TIME STEP = <real>target_time_step}

command line or an

\texttt{ALLOWABLE MASS INCREASE RATIO = <real>mass_increase_ratio}

command line, or both of these command lines can appear in the input block.

The TARGET TIME STEP command lines sets the maximum time step for a set of nodes. The parameter target_time_step is the maximum time step for all the nodes specified in the command block.

The ALLOWABLE MASS INCREASE RATIO command line sets an upper limit on the mass scaling at a node. The value specified for mass_increase_ratio limits the ratio of the mass at a node, as set by mass scaling, to the original mass at the node. (The original mass of the node is determined only by the element contributions.) This ratio must be a factor greater than or equal to 1. If \( m_s \) is the scaled mass at a node and \( m_0 \) is the original mass at the node due only to element contributions, then the ratio \( m_s / m_0 \) will not exceed the value of mass_increase_ratio.

Mass scaling will add mass to nodes until the target time step is reached, the mass added to some node reaches the allowable mass increase ratio, or the current set of nodes no longer controls the global analysis time step.

The amount of mass added due to mass scaling is stored in the nodal variable mass_scaling_added_mass. This variable can be output and postprocessed to determine how much mass is being added at a given time. See Section 8.1.1 regarding the output of nodal variables to a results file.
3.3.3 Additional Command

The `ACTIVE PERIODS` command line can appear as an option in the `MASS SCALING` command block:

```
ACTIVE PERIODS = <string list>periods
```

This command line determines when mass scaling is active. See Section 2.5 for more information about this command line.
3.4 References


Chapter 4

Materials

This chapter describes material models that can be used in conjunction with the elements in Presto and Adagio. Most of the material models have an interface that allows them to be used by the elements in both codes. Even though a material model can be used by both codes, usage of the model may be better suited for the type of problems solved by one code rather than the type of problems solved by the other code. For example, a material model that was built to characterize behavior over a long time would be better suited for use in Adagio than in Presto. If a particular material model is better suited for one code rather than the other, this usage information is provided in the description of that model. Furthermore, there is a class of material models that are referred to as equation-of-state models. These models are designed for an explicit, transient dynamics code, and, as such are applicable only for use in Presto. Hence, descriptions of the equation-of-state models and any associated calculations that are used with these models, such as energy deposition, are included in the chapter on material models in the Presto user’s guide but not in the corresponding chapter on material models of the Adagio user’s guide.

The material models described in this chapter are, in general, applicable to solid elements. The structural elements, such as shells and beams, have a much more limited set of material models. You should consult with Chapter 5, which discusses the element library, to determine what material models are available for the various elements. The introduction to Chapter 5 summarizes all the element types in Presto and Adagio. For each element type, a list of available material models is provided.

When using the nonlinear material models, you may want to output state variables that are associated with these models. See Section 8.6.2 to learn how to output the state variables for the various nonlinear material models.

Most material models for solid elements are available in two libraries. The newer library is the LAME library [12], but it is not the default. The line command to activate the LAME material library for a particular section is described in Section 5.2.1.

**General Model Form.** PROPERTY SPECIFICATION FOR MATERIAL command blocks appear in the domain scope in the general form shown below.

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
```
PROPERTY SPECIFICATION FOR MATERIAL command blocks are physics independent in the sense that the information in them can be shared by more than one application. For example, some of the PROPERTY SPECIFICATION FOR MATERIAL command blocks contain density information that can be shared among several applications.

The command block begins with an input line of the form:

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name

and is terminated with an input line of the following form:

END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

Here, the string mat_name is a user-specified name for the command block. This name is typically descriptive of the material being modeled, e.g., aluminum_t6061.

Within a PROPERTY SPECIFICATION FOR MATERIAL command block, there will be other command blocks and possibly other general material command lines that are used to describe particular material models. The general material command lines, if present, are listed first, followed by one or more material-model command blocks. The general material command lines may be used to specify the density of the material as well as the application of temperatures and thermal strains to two- or three-dimensional elements. Each material-model command block follows the naming convention of PARAMETERS FOR MODEL model_name, where model_name identifies a particular material model, such as elastic, elastic-plastic, or orthotropic crush. Each such command block contains all the parameters needed to describe a particular material model.

As noted above, more than one material-model command block can appear within a PROPERTY SPECIFICATION FOR MATERIAL command block. Suppose we have a PROPERTY SPECIFICATION FOR MATERIAL command block called steel. It would be possible to have two material-model command blocks within this command block. One of the material-model command blocks would provide an elastic model for steel; the other material-model command block would provide an elastic-plastic model for steel. The general form of a PROPERTY SPECIFICATION FOR MATERIAL command block would be as follows:
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name

# {General material command lines}
DENSITY = <real>density_value

# THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
  <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
  <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
  <string>thermal_strain_z_function

# BEGIN PARAMETERS FOR MODEL <string>model_name1
  {Parameters for material model model_name1}
END PARAMETERS FOR MODEL <string>model_name1

# BEGIN PARAMETERS FOR MODEL <string> model_name2
  {Parameters for material model model_name2}
END PARAMETERS FOR MODEL <string> model_name2

{Additional model command blocks if required}

# END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

In the above general form for a PROPERTY SPECIFICATION FOR MATERIAL command block, the string model_name1 could be ELASTIC and the string model_name2 could be ORTHOTROPIC CRUSH. Typically, however, only one material model would be desired for a given block, and the PROPERTY SPECIFICATION FOR MATERIAL command block would have only one PARAMETERS FOR MODEL command block. A particular material model may only appear once within a given PROPERTY SPECIFICATION FOR MATERIAL command block.

Although multiple material models can be defined for one material within a PROPERTY Specification FOR MATERIAL command block, only one material model is actually used for a given element block during an analysis. The ability to define multiple constitutive models for one material is provided as a convenience to enable the user to easily switch between models. The material name and the model name are both referenced when material models are assigned to element blocks within the FINITE ELEMENT MODEL command block, which is described in Section 5.1.

This chapter, in general, is organized to correspond to the general form presented for the PROPERTY SPECIFICATION FOR MATERIAL command block. Section 4.1 discusses the DENSITY command line and the command lines used for thermal strains, and also explains how temperatures and thermal strains are applied. Section 4.2 describes each of the material models that are shared by Presto and Adagio. Section 4.3 describes the equation-of-state material models, which are used only in Presto. Section 4.4 presents the contents of the ENERGY DEPOSITION command block, which also is only used in Presto. Energy deposition is used only in conjunction with the equation-of-state material models. Although energy deposition is not an element-like functionality (but
rather a “boundary condition”-like functionality), it is most convenient to include the description of energy deposition with the equation-of-state material models. References applicable for both Presto and Adagio are listed in Section 4.5.

As indicated in the introductory material, not all the material models available are applicable to all the element types. As one example, there is a one-dimensional elastic material model that is used for a truss element but is not applicable to solid elements such as hexahedra or tetrahedra. For this particular example, the specific material-model usage is hidden from the user. If the user specifies a linear elastic material model for a truss, the one-dimensional elastic material model is used. If the user specifies a linear elastic material model for a hexahedron, a full three-dimensional elastic material model is used. As another example, the energy-dependent material models available in Presto cannot be used for a one-dimensional element such as a truss. The energy-dependent material models can only be used for solid elements such as hexahedra and tetrahedra. (Chapter 5 indicates what material models are available for which element models.)

For each material model, the parameters needed to describe that model are listed in the section pertinent to that particular model. Solid models with elastic constants require only two elastic constants. These two constants are then used to generate all the elastic constants for the model. For example, if the user specifies Young’s modulus and Poisson’s ratio, then the shear modulus, bulk modulus, and lambda are calculated. If the shear modulus and lambda are specified, then Young’s modulus, Poisson’s ratio, and the bulk modulus are calculated.

The various nonlinear material models have state variables. See Section 8.6.2 to learn how to output the state variables for the nonlinear material models.

Note that only brief descriptions of the material models are presented in this chapter. For a detailed description of the various material models, you will need to consult a variety of references. Specific references are identified for most of the material models shared by Presto and Adagio. The references for the equation-of-state material models appear in both the Presto and Adagio user guides, even though information about the equation-of-state models appears only in the Presto user’s guide.
4.1 General Material Commands

A PROPERTY SPECIFICATION FOR MATERIAL command block for a particular material may include additional command lines that are applicable to all the material models specified within the command block. These command lines related to density and to thermal strain behavior are discussed, respectively, in Section 4.1.1 and Section 4.1.2.

4.1.1 Density Command

DENSITY = <real>density_value

This command line specifies the density of the material described in a PROPERTY SPECIFICATION FOR MATERIAL command block. The units of the input parameter density_value are specified as mass per unit volume.

As previously explained, a PROPERTY SPECIFICATION FOR MATERIAL command block can contain one or more PARAMETERS FOR MODEL command blocks. The specified density_value for the material will be used with all of the models described in these PARAMETERS FOR MODEL command blocks.

4.1.2 Thermal Strain Behavior

Isotropic and orthotropic thermal strains may be defined for use by material models listed in a PROPERTY SPECIFICATION FOR MATERIAL command block. Section 4.1.2.1 describes the command lines that are used to define the thermal strain behavior. These command lines must be used in conjunction with other command blocks outside of a PROPERTY SPECIFICATION FOR MATERIAL command block for the calculations of thermal strains to be activated. Section 4.1.2.2 explains the process for activating thermal strains.

4.1.2.1 Defining Thermal Strains

THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
<string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
<string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
<string>thermal_strain_z_function

A PROPERTY SPECIFICATION FOR MATERIAL command block may include command lines that define thermal strain behavior. It is possible to specify either an isotropic thermal-strain field
using the command line THERMAL STRAIN FUNCTION or an orthotropic thermal-strain field using the command lines THERMAL STRAIN X FUNCTION, THERMAL STRAIN Y FUNCTION, and THERMAL STRAIN Z FUNCTION. For any of these command lines, the user supplies a thermal strain function (via a DEFINITION FOR FUNCTION command block), which defines the thermal strain as a function of temperature. The computed thermal strain is then subtracted from the strain passed to the material model.

A thermal strain can be applied to any two-dimensional or three-dimensional element, regardless of material type. For a three-dimensional element such as a hexahedron or tetrahedron, the thermal strains are applied to the strain in the global XYZ coordinate system. For the isotropic case, the thermal strains are the same in the X-direction, the Y-direction, and the Z-direction. For the anisotropic case, the thermal strains can be different in each of the three global directions—X, Y, and Z. For a two-dimensional element, shell or membrane, the thermal strain corresponding to the THERMAL STRAIN X FUNCTION command line is applied to the strain in the shell (or membrane) r-direction. (Reference Section 5.2.2 for a discussion of the shell rst coordinate system.) The thermal strain corresponding to the THERMAL STRAIN Y FUNCTION command line is applied to the strain in the shell (or membrane) s-direction. For two-dimensional elements, the current implementation of orthotropic thermal strains is limited, for practical purposes, to special cases—flat sheets of uniform shell elements lying in one of the global planes, e.g., XY, YZ, or ZX. The current orthotropic thermal-strain capability has limited use for shells and membranes in the current release of the code. Tying the orthotropic thermal-strain functionality to the shell orientation functionality (Section 5.2.2) in the future will provide much more useful orthotropic thermal-strain functionality for two-dimensional elements.

If an isotropic thermal-strain field is to be applied, the THERMAL STRAIN FUNCTION command line is placed in the PROPERTY SPECIFICATION FOR MATERIAL command block, outside of the specifications of any material models in the block. Such placement is necessary because the isotropic thermal strain is a general material property, not a property that is specific to any particular constitutive model, such as ELASTIC or ELASTIC-PLASTIC. The input value of thermal_strain_function is the name of the function that defines thermal strain as a function of temperature for the material model described in this particular PROPERTY SPECIFICATION FOR MATERIAL command block. The function is defined within the domain scope using a DEFINITION FOR FUNCTION command block. For more information on how to set the input to compute thermal strains and how to apply temperatures, see Section 4.1.2.2.

The specification of an orthotropic thermal-strain field requires that all three of the THERMAL STRAIN X FUNCTION, THERMAL STRAIN Y FUNCTION, and THERMAL STRAIN Z FUNCTION command lines be placed in the PROPERTY SPECIFICATION FOR MATERIAL command block. All three command lines must be provided, even when there is no thermal strain in one or more directions. The values of thermal_strain_x_function, thermal_strain_y_function, and thermal_strain_z_function are the names of the functions for thermal strains in the X-direction, the Y-direction, and the Z-direction, respectively. These functions are defined within the domain scope using DEFINITION FOR FUNCTION command blocks. To specify that there should be no thermal strain in a given direction, use a function that always evaluates to zero for that direction.
The THERMAL STRAIN FUNCTION command line and the THERMAL STRAIN X FUNCTION, THERMAL STRAIN Y FUNCTION, and THERMAL STRAIN Z FUNCTION command lines are not used for several of the material models, as discussed in Section 4.1.2.2. Note that specification of a thermal strain is identified in the descriptions of the material models in Section 4.2 by the notation “{thermal strain option}”.
4.1.2.2 Activating Thermal Strains

Presto has the capability to compute thermal strains on three-dimensional continuum and two-dimensional (shell, membrane) elements. Three things are required to activate thermal strains:

- First, one or more thermal strain functions (strain as a function of temperature) must be defined. Each thermal strain function is defined with a `DEFINITION FOR FUNCTION` command block. (This function is the standard function definition that appears in the domain scope.) The thermal strain function gives the total thermal strain associated with a given temperature. It is the change in thermal strain with the change in temperature that gives rise to thermal stresses in a body.

- Second, the material models used by blocks that experience thermal strain must have their thermal strain behavior defined. The command lines for defining isotropic and orthotropic thermal strain are described in Section 4.1.2.1. Materials with isotropic thermal strain use the `THERMAL STRAIN FUNCTION` command line, while those with orthotropic thermal strain must define thermal strain in all three directions using the `THERMAL STRAIN X FUNCTION`, `THERMAL STRAIN Y FUNCTION`, and `THERMAL STRAIN Z FUNCTION` command lines. These inputs can be used with all material models with the exception of the following: elastic three-dimensional orthotropic, elastic laminate, Mooney-Rivlin, NLVE three-dimensional orthotropic, Swanson, and viscoelastic Swanson. These models require their own model-specific inputs to define thermal strain and must not use these standard commands. Information for defining thermal strains is provided in the individual descriptions of these models in Section 4.2.

- Third, a temperature field must be applied to the affected blocks. The command block to specify the application of temperatures is `PRESCRIBED TEMPERATURE`, which is implemented as a standard boundary condition. A description of the `PRESCRIBED TEMPERATURE` command block is given in Section 6.7.

Whenever a temperature field is applied, the temperature is prescribed at the nodes, but thermal strain is computed based on element temperature. Element temperatures are obtained by averaging the temperatures of the nodes connected to a given element. Thermal strains are applied in rate form, so the thermal strain in an element is relative to the thermal strain at the initial temperature. Thus, the initial temperature is the stress-free temperature. If desired, a different stress-free temperature can be used by prescribing the initial temperature with the `INITIAL CONDITION` command block as described in Section 6.2.
4.2 Model Specifications

This section contains descriptions of the material models that are shared by Presto and Adagio.
4.2.1 Elastic Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
<string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
<string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
<string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL ELASTIC
  YOUNGS MODULUS = <real>youngs_modulus
  POISSONS RATIO = <real>poissons_ratio
  SHEAR MODULUS = <real>shear_modulus
  BULK MODULUS = <real>bulk_modulus
  LAMBDA = <real>lambda
END [PARAMETERS FOR MODEL ELASTIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

An elastic material model is used to describe simple linear elastic behavior of materials. This model is generally valid for small deformations.

For an elastic material, an elastic command block starts with the input line:

BEGIN PARAMETERS FOR MODEL ELASTIC

and terminates with an input line of the following form:

END [PARAMETERS FOR MODEL ELASTIC]

In the above command blocks:

- The density of the material is defined with the DENSITY command line.

- The {thermal strain option} is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.

- Only two of the following elastic constants are required:
  
  - Young’s modulus is defined with the YOUNGS MODULUS command line.
  - Poisson’s ratio is defined with the POISSONS RATIO command line.
  - The bulk modulus is defined with the BULK MODULUS command line.
  - The shear modulus is defined with the SHEAR MODULUS command line.
• Lambda is defined with the LAMBDA command line.

For information about the elastic model, consult Reference 1.
4.2.2 Elastic Fracture Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  # {thermal strain option}
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL ELASTIC_FRACTURE
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    MAX STRESS = <real>max_stress
    CRITICAL STRAIN = <real>critical_strain
  END [PARAMETERS FOR MODEL ELASTIC_FRACTURE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

An elastic fracture material is a simple failure model that is based on linear elastic behavior. The model uses a maximum-principal-stress failure criterion. The stress decays isotropically based on the component of strain parallel to the maximum principal stress. The value of the component of strain over which the stress is decayed to zero is a user-defined parameter for the model. This strain parameter can be adjusted so that failure is mesh independent.

For an elastic fracture material, an elastic fracture command block starts with the input line:

BEGIN PARAMETERS FOR MODEL ELASTIC_FRACTURE

and terminates with an input line of the following form:

END [PARAMETERS FOR MODEL ELASTIC_FRACTURE]

In the above command blocks:

- The density of the material is defined with the DENSITY command line.

- The {thermal strain option} is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.

- Only two of the following elastic constants are required:

  - Young’s modulus is defined with the YOUNGS MODULUS command line.
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- Poisson’s ratio is defined with the POISSONS RATIO command line.
- The bulk modulus is defined with the BULK MODULUS command line.
- The shear modulus is defined with the SHEAR MODULUS command line.
- Lambda is defined with the LAMBDA command line.

- The maximum principal stress at which failure occurs is defined with the MAX STRESS command line.

- The component of strain over which the stress decays to zero is defined with the CRITICAL STRAIN command line. This component of strain is aligned with the maximum-principal-stress direction at failure.
4.2.3 Elastic-Plastic Model

ettings for a material, an elastic-plastic command block starts with the input line:

```
BEGIN PARAMETERS FOR MODEL ELASTIC_PLASTIC
```

and terminates with an input line of the following form:

```
END [PARAMETERS FOR MODEL ELASTIC_PLASTIC]
```

In the above command blocks:

The elastic-plastic linear hardening models are used to model materials, typically metals, that undergo plastic deformation at finite strains. Linear hardening generally refers to the shape of a uniaxial stress-strain curve where the stress increases linearly with the plastic, or permanent, strain. In a three-dimensional framework, hardening is the law that governs how the yield surface grows in stress space. If the yield surface grows uniformly in stress space, the hardening is referred to as isotropic hardening. When `BETA` is 1.0, we have only isotropic hardening.

Because the linear hardening model is relatively simple to integrate, the model also has the ability to define a yield surface that not only grows, or hardens, but also moves in stress space. This ability is known as kinematic hardening. When `BETA` is 0.0, we have only kinematic hardening. The elastic-plastic linear hardening model allows for isotropic hardening, kinematic hardening, or a combination of the two.

For an elastic-plastic material, an elastic-plastic command block starts with the input line:

```
BEGIN PARAMETERS FOR MODEL ELASTIC_PLASTIC
```

and terminates with an input line of the following form:

```
END [PARAMETERS FOR MODEL ELASTIC_PLASTIC]
```

In the above command blocks:
- The density of the material is defined with the `DENSITY` command line.

- The `{thermal strain option}` is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.

- Only two of the following elastic constants are required:
  
  - Young’s modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson’s ratio is defined with the `POISONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.

- The yield stress is defined with the `YIELD STRESS` command line.

- The hardening modulus is defined with the `HARDENING MODULUS` command line.

- The beta parameter is defined with the `BETA` command line.

For information about the elastic-plastic model, consult Reference 1.
4.2.4 Elastic-Plastic Power-Law Hardening Model

A power-law hardening model for elastic-plastic materials is used for modeling metal plasticity up to finite strains. The power-law hardening model, as opposed to the linear hardening model, has a power law fit for the uniaxial stress-strain curve that has the stress increase as the plastic strain raised to some power. The power-law hardening model also has the ability to model materials that exhibit Luder’s strains after yield. Due to the more complicated yield behavior, the power-law hardening model can only be used with isotropic hardening.

For an elastic-plastic power-law hardening material, an elastic-plastic power-law hardening command block starts with the input line:

```
BEGIN PARAMETERS FOR MODEL EP_POWER_HARD
```

and terminates with an input line of the following form:

```
END [PARAMETERS FOR MODEL EP_POWER_HARD]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The `{thermal strain option}` is used to define thermal strains. See Section 4.1.2.1.
and Section 4.1.2.2 for further information on specifying and applying thermal strains and temperatures.

- Only two of the following elastic constants are required:
  
  - Young’s modulus is defined with the YOUNGS MODULUS command line.
  - Poisson’s ratio is defined with the POISSONS RATIO command line.
  - The bulk modulus is defined with the BULK MODULUS command line.
  - The shear modulus is defined with the SHEAR MODULUS command line.
  - Lambda is defined with the LAMBDA command line.

- The yield stress is defined with the YIELD STRESS command line.

- The hardening constant is defined with the HARDENING CONSTANT command line.

- The hardening exponent is defined with the HARDENING EXPONENT command line.

- The Luder’s strain is defined with the LUDERS STRAIN command line.

For information about the elastic-plastic power-law hardening model, consult Reference 1.
4.2.5 Ductile Fracture Model

This model is identical to the elastic-plastic power-law hardening model with the addition of a failure criterion and a postfailure isotropic decay of the stress to zero within the constitutive model. The point at which failure occurs is defined by a critical tearing parameter. The critical tearing parameter \( t_p \) is related to the plastic strain at failure \( \varepsilon_f \) by the evolution integral

\[
t_p = \int_0^{\varepsilon_f} \left( \frac{2\sigma_{\text{max}}}{3(\sigma_{\text{max}} - \sigma_m)} \right)^4 \varepsilon_p \, d\varepsilon_p.
\]  

(4.1)

In Equation (4.1), \( \sigma_{\text{max}} \) is the maximum principal stress, and \( \sigma_m \) is the mean stress. The quantity in the angle brackets, the expression

\[
\frac{2\sigma_{\text{max}}}{3(\sigma_{\text{max}} - \sigma_m)},
\]  

(4.2)

is nonzero only if it evaluates to a positive value. This quantity is set to zero if it has a negative value.

The stress decays isotropically based on the component of strain parallel to the maximum principal stress. The value of the component of strain over which the stress is decayed to zero is a user-
defined parameter for the model. This strain parameter can be adjusted so that failure is mesh independent.

For an elastic-plastic power-law hardening material with failure, the command block starts with the input line:

```
BEGIN PARAMETERS FOR MODEL DUCTILE_FRACTURE
```

and terminates with an input line of the following form:

```
END [PARAMETERS FOR MODEL DUCTILE_FRACTURE]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The `{thermal strain option}` is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains and temperatures.
- Only two of the following elastic constants are required:
  - Young’s modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson’s ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The yield stress is defined with the `YIELD STRESS` command line.
- The hardening constant is defined with the `HARDENING CONSTANT` command line.
- The hardening exponent is defined with the `HARDENING EXPONENT` command line.
- The Luder’s strain is defined with the `LUDERS STRAIN` command line.
- The critical tearing parameter is defined with the `CRITICAL TEARING PARAMETER` command line.
- The component of strain over which the stress decays to zero is defined with the `CRITICAL CRACK OPENING STRAIN` command line. This component of strain is aligned with the maximum-principal-stress direction at failure.

For information about the ductile fracture material model, consult Reference 1.
4.2.6 Multilinear Elastic-Plastic Hardening Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
#
# or all three of the following
THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL MULTILINEAR_EP
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    BETA = <real>betta_parameter(1.0)
    HARDENING FUNCTION = <real>hardening_function_name
    YOUNGS MODULUS FUNCTION = <real>ym_function_name
    POISSONS RATIO FUNCTION = <real>pr_function_name
    YIELD STRESS FUNCTION = <real>yield_stress_function_name
END [PARAMETERS FOR MODEL MULTILINEAR_EP]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

This model is similar to the power-law hardening model except that the hardening behavior is described with a piecewise-linear curve as opposed to a power law.

For a multilinear elastic-plastic hardening material, the command block starts with the input line:

BEGIN PARAMETERS FOR MODEL MULTILINEAR_EP

and terminates with an input line of the following form:

END [PARAMETERS FOR MODEL MULTILINEAR_EP]

In the above command blocks:

- The density of the material is defined with the DENSITY command line.

- The {thermal strain option} is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.

- Only two of the following elastic constants are required:
4.2. MODEL SPECIFICATIONS

- Young’s modulus is defined with the `YOUNGS MODULUS` command line.
- Poisson’s ratio is defined with the `POISSONS RATIO` command line.
- The bulk modulus is defined with the `BULK MODULUS` command line.
- The shear modulus is defined with the `SHEAR MODULUS` command line.
- Lambda is defined with the `LAMBD A` command line.

- The yield stress is defined with the `YIELD STRESS` command line.

- The beta parameter is defined with the `BETA` command line.

- The `HARDENING FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the domain scope that describes the hardening behavior of the material as a stress versus equivalent plastic strain. This curve is expressed as the additional increment of stress over the yield stress versus equivalent plastic strain, thus the first point on the curve should be (0.0, 0.0).

- The `YOUNGS MODULUS FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the domain scope that describes a scale factor on Young’s modulus as a function of temperature.

- The `POISSONS RATIO FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the domain scope that describes a scale factor on Poisson’s ratio as a function of temperature.

- The `YIELD STRESS FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the domain scope that describes a scale factor on the yield stress as a function of temperature.
4.2.7 Multilinear Elastic-Plastic Hardening Model with Failure

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
<string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
<string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
<string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL ML_EP_FAIL
YOUNGS MODULUS = <real>youngs_modulus
POISSONS RATIO = <real>poissons_ratio
SHEAR MODULUS = <real>shear_modulus
BULK MODULUS = <real>bulk_modulus
LAMBDA = <real>lambda
YIELD STRESS = <real>yield_stress
BETA = <real>beta_parameter(1.0)
HARDENING FUNCTION = <real>hardening_function_name
YOUNGS MODULUS FUNCTION = <real>ym_function_name
POISSONS RATIO FUNCTION = <real>pr_function_name
YIELD STRESS FUNCTION = <real>yield_stress_function_name
CRITICAL TEARING PARAMETER = <real>crit_tearing
CRITICAL CRACK OPENING STRAIN = <real>crit_crack
END [PARAMETERS FOR MODEL ML_EP_FAIL]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

This model is similar to the power-law hardening model except that the hardening behavior is described with a piecewise-linear curve as opposed to a power law. This model incorporates a failure criterion and a postfailure isotropic decay of the stress to zero within the constitutive model. The point at which failure occurs is defined by a critical tearing parameter. The critical tearing parameter $t_p$ is related to the plastic strain at failure $\varepsilon_f$ by the evolution integral:

$$ t_p = \int_0^{\varepsilon_f} \left\langle \frac{2\sigma_{\text{max}}}{3(\sigma_{\text{max}} - \sigma_{m})} \right\rangle^4 \, d\varepsilon_p. \quad (4.3) $$

In Equation (4.3), $\sigma_{\text{max}}$ is the maximum principal stress, and $\sigma_{m}$ is the mean stress. The quantity in the angle brackets, the expression

$$ \frac{2\sigma_{\text{max}}}{3(\sigma_{\text{max}} - \sigma_{m})}, \quad (4.4) $$

is nonzero only if it evaluates to a positive value. This quantity is set to zero if it has a negative value.
The stress decays isotropically based on the component of strain parallel to the maximum principal stress. The value of the component of strain over which the stress is decayed to zero is a user-defined parameter for the model. This strain parameter can be adjusted so that failure is mesh independent.

For a multilinear elastic-plastic hardening material with failure, the command block starts with the input line

```
BEGIN PARAMETERS FOR MODEL ML_EP_FAIL
```

and terminates with an input line of the following form:

```
END [PARAMETERS FOR MODEL ML_EP_FAIL]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The `{thermal strain option}` is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.
- Only two of the following elastic constants are required:
  - Young’s modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson’s ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.
- The yield stress is defined with the `YIELD STRESS` command line.
- The beta parameter is defined with the `BETA` command line.
- The `HARDENING FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the domain scope that describes the hardening behavior of the material as a stress versus equivalent plastic strain. This curve is expressed as the additional increment of stress over the yield stress versus equivalent plastic strain, thus the first point on the curve should be (0.0, 0.0).
- The `YOUNGS MODULUS FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the domain scope that describes a scale factor on Young’s modulus as a function of temperature.
- The `POISSONS RATIO FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the domain scope that describes a scale factor on Poisson’s ratio as a function of temperature.
- The `YIELD STRESS FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the domain scope that describes a scale factor on the yield stress as a function of temperature.
- The critical tearing parameter is defined with the `CRITICAL TEARING PARAMETER` command line.

- The component of strain over which the stress decays to zero is defined with the `CRITICAL CRACK OPENING STRAIN` command line. This component of strain is aligned with the maximum-principal-stress direction at failure.
4.2.8 Johnson-Cook Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
    DENSITY = <real>density_value
    #
    # {thermal strain option}
    THERMAL STRAIN FUNCTION = <string>thermal_strain_function
    # or all three of the following
    THERMAL STRAIN X FUNCTION =
        <string>thermal_strain_x_function
    THERMAL STRAIN Y FUNCTION =
        <string>thermal_strain_y_function
    THERMAL STRAIN Z FUNCTION =
        <string>thermal_strain_z_function
    #
    BEGIN PARAMETERS FOR MODEL JOHNSON_COOK
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    YIELD STRESS = <real>yield_stress
    HARDENING CONSTANT = <real>hardening_constant
    HARDENING EXPONENT = <real>hardening_exponent
    RHOCV = <real>rho_cv
    RATE CONSTANT = <real>rate_constant
    THERMAL EXPONENT = <real>thermal_exponent
    REFERENCE TEMPERATURE = <real>reference_temperature
    MELT TEMPERATURE = <real>melt_temperature
    END [PARAMETERS FOR MODEL JOHNSON_COOK]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

The Johnson-Cook model is used to model materials, typically metals, that undergoing plastic deformation at finite strains.

BEGIN PARAMETERS FOR MODEL JOHNSON_COOK
and terminates with an input line of the following form:

END [PARAMETERS FOR MODEL JOHNSON_COOK]

In the above command blocks:

- The density of the material is defined with the DENSITY command line.

- The {thermal strain option} is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.

- Only two of the following elastic constants are required:
- Young’s modulus is defined with the \texttt{YOUNGS MODULUS} command line.
- Poisson’s ratio is defined with the \texttt{POISSONS RATIO} command line.
- The bulk modulus is defined with the \texttt{BULK MODULUS} command line.
- The shear modulus is defined with the \texttt{SHEAR MODULUS} command line.
- Lambda is defined with the \texttt{LAMBDA} command line.

- The yield stress is defined with the \texttt{YIELD STRESS} command line.
- The hardening constant is defined with the \texttt{HARDENING CONSTANT} command line.
- The hardening exponent is defined with the \texttt{HARDENING EXPONENT} command line.
- The rhocv is defined with the \texttt{RHOCV} command line.
- The thermal exponent is defined with the \texttt{THERMAL EXPONENT} command line.
- The reference temperature is defined with the \texttt{REFERENCE TEMPERATURE} command line.
- The melt temperature is defined with the \texttt{MELT TEMPERATURE} command line.

For information about the Johnson-Cook material model, consult Reference 17.
4.2. MODEL SPECIFICATIONS

4.2.9 BCJ Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  #
  # {thermal strain option}
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
BEGIN PARAMETERS FOR MODEL BCJ
  YOUNGS MODULUS = <real>youngs_modulus
  POISSONS RATIO = <real>poissons_ratio
  SHEAR MODULUS = <real>shear_modulus
  BULK MODULUS = <real>bulk_modulus
  LAMBDA = <real>lambda
  C1 = <real>c1
  C2 = <real>c2
  C3 = <real>c3
  C4 = <real>c4
  C5 = <real>c5
  C6 = <real>c6
  C7 = <real>c7
  C8 = <real>c8
  C9 = <real>c9
  C10 = <real>c10
  C11 = <real>c11
  C12 = <real>c12
  C13 = <real>c13
  C14 = <real>c14
  C15 = <real>c15
  C16 = <real>c16
  C17 = <real>c17
  C18 = <real>c18
  C19 = <real>c19
  C20 = <real>c20
  DAMAGE EXPONENT = <real>damage_exponent
  INITIAL ALPHA_XX = <real>alpha_xx
  INITIAL ALPHA YY = <real>alpha_yy
  INITIAL ALPHA ZZ = <real>alpha_zy
  INITIAL ALPHA XY = <real>alpha_xy
  INITIAL ALPHA YZ = <real>alpha_yz
The BCJ plasticity model is a state-variable model for describing the finite deformation behavior of metals. It uses a multiplicative decomposition of the deformation gradient into elastic, volumetric plastic, and deviatoric parts. The model considers the natural configuration defined by this decomposition and its associated thermodynamics. The model incorporates strain rate and temperature sensitivity, as well as damage, through a yield-surface approach in which state variables follow a hardening-minus-recovery format.

Because the BCJ model has such an extensive list of parameters, we will not present the usual synopsis of parameter names with command lines. As with most other material models, the {thermal strain option} is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains. In addition, only two of the five elastic constants are required. The user should consult References 2, 3, and 4 for a description of the various parameters. Note that the parameters for the SPECIFIC HEAT, THETA OPT, FACTOR, RHO, and TEMP0 command lines are used to accommodate changes to the model for heat generation due to plastic dissipation. For coupled solid/thermal calculations, the plastic dissipation rate is stored as a state variable and passed to a thermal code as a heat source term. For uncoupled calculations, temperature is stored as a state variable, and temperature increases due to plastic dissipation are calculated within the material model.

If temperature is provided from an external source, \texttt{theta\_opt} is set to 0. If the temperature is calculated by the BCJ model, \texttt{theta\_opt} is set to 1.
4.2.10 Soil and Crushable Foam Model

**BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name**

DENSITY = <real>density_value

# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function

# or all three of the following
THERMAL STRAIN X FUNCTION = <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION = <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION = <string>thermal_strain_z_function

#
BEGIN PARAMETERS FOR MODEL SOIL_FOAM

YOUNGS MODULUS = <real>youngs_modulus
POISSONS RATIO = <real>poissons_ratio
SHEAR MODULUS = <real>shear_modulus
BULK MODULUS = <real>bulk_modulus
LAMBDA = <real>lambda
A0 = <real>const_coeff_yieldsurf
A1 = <real>lin_coeff_yieldsurf
A2 = <real>quad_coeff_yieldsurf
PRESSURE CUTOFF = <real>pressure_cutoff
PRESSURE FUNCTION = <string>function_press_volstrain

END [PARAMETERS FOR MODEL SOIL_FOAM]

END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

The soil and crushable foam model is a plasticity model that can be used for modeling soil or crushable foam. Given the right input, the model is a Drucker-Prager model.

For the soil and crushable foam model, the yield surface is a surface of revolution about the hydrostat in principal stress space. A planar end cap is assumed for the yield surface so that the yield surface is closed. The yield stress $\sigma_{yd}$ is specified as a polynomial in pressure $p$. The yield stress is given as:

$$\sigma_{yd} = a_0 + a_1 p + a_2 p^2,$$  \hspace{1cm} (4.5)

where $p$ is positive in compression. The determination of the yield stress from Equation (4.5) places severe restrictions on the admissible values of $a_0$, $a_1$, and $a_2$. There are three valid cases for the yield surface. In the first case, there is an elastic–perfectly plastic deviatoric response, and the yield surface is a cylinder oriented along the hydrostat in principal stress space. In this case, $a_0$ is positive, and $a_1$ and $a_2$ are zero. In the second case, the yield surface is conical. A conical yield surface is obtained by setting $a_2$ to zero and using appropriate values for $a_0$ and $a_1$. In the third case, the yield surface has a parabolic shape. For the parabolic yield surface, all three coefficients
in Equation (4.5) are nonzero. The coefficients are checked to determine that a valid negative
ten
sile-failure pressure can be derived based on the specified coefficients.

For the case of the cylindrical yield surface (e.g., $a_0 > 0$ and $a_1 = a_2 = 0$), there is no tensile-failure
pressure. For the other two cases, the computed tensile-failure pressure may be too low. To handle
the situations where there is no tensile-failure pressure or the tensile-failure pressure is too low,
a pressure cutoff can be defined. If a pressure cutoff is defined, the tensile-failure pressure is the
larger of the computed tensile-failure pressure and the defined cutoff pressure.

The plasticity theories for the volumetric and deviatoric parts of the material response are com-
pletely uncoupled. The volumetric response is computed first. The mean pressure $p$ is assumed to
be positive in compression, and a yield function $\phi_p$ is written for the volumetric response as:

$$\phi_p = p - f_p(\varepsilon_V), \quad (4.6)$$

where $f_p(\varepsilon_V)$ defines the volumetric stress-strain curve for the pressure. The yield function $\phi_p$
determines the motion of the end cap along the hydrostat.

For a soil and crushable foam material, a soil and crushable foam command block starts with the
input line:

```
BEGIN PARAMETERS FOR MODEL SOIL_FOAM
```

and terminates with an input line of the following form:

```
END [PARAMETERS FOR MODEL SOIL_FOAM]
```

In the above command blocks:

- The density of the material is defined with the DENSITY command line.
- The {thermal strain option} is used to define thermal strains. See Section 4.1.2.1 and
  Section 4.1.2.2 for further information on defining and activating thermal strains.
- Only two of the following elastic constants are required:
  - Young’s modulus is defined with the YOUNG’S MODULUS command line.
  - Poisson’s ratio is defined with the POISSON’S RATIO command line.
  - The bulk modulus is defined with the BULK MODULUS command line.
  - The shear modulus is defined with the SHEAR MODULUS command line.
  - Lambda is defined with the LAMBDA command line.
- The constant in the equation for the yield surface is defined with the A0 command line.
- The coefficient for the linear term in the equation for the yield surface is defined with the A1
  command line.
- The coefficient for the quadratic term in the equation for the yield surface is defined with the
  A2 command line.
4.2. MODEL SPECIFICATIONS

- The user-defined tensile-failure pressure is defined with the `PRESSURE_CUTOFF` command line.

- The pressure as a function of volumetric strain is defined with the function named on the `PRESSURE_FUNCTION` command line.

For information about the soil and crushable foam model, consult with the Pronto3d document listed as Reference 5. The soil and crushable foam model is the same as the soil and crushable foam model in Pronto3d. The Pronto3d model is based on a material model developed by Krieg [6]. The Krieg version of the soil and crushable foam model was later modified by Swenson and Taylor [7]. The soil and crushable foam model developed by Swenson and Taylor is the model in Pronto3d and is also the shared model for Presto and Adagio.
CHAPTER 4. MATERIALS

4.2.11 Foam Plasticity Model

The foam plasticity model was developed to describe the response of porous elastic-plastic materials like closed-cell polyurethane foam to large deformation. Like solid metals, these foams can exhibit significant plastic deviatoric strains (permanent shape changes). Unlike metals, these foams can also exhibit significant plastic volume strains (permanent volume changes). The foam plasticity model is characterized by an initial yield surface that is an ellipsoid about the hydrostat.

When foams are compressed, they typically exhibit an initial elastic regime followed by a plateau regime in which the stress needed to compress the foam remains nearly constant. At some point in the compression process, the densification regime is reached, and the stress needed to compress the foam further begins to rapidly increase.

The foam plasticity model can be used to describe the response of metal foams and many closed-cell polymeric foams (including polyurethane, polystyrene bead, etc.) subjected to large deformation. This model is not appropriate for flexible foams that return to their undeformed shape after loads are removed.
For a foam plasticity material, a foam plasticity command block starts with the input line:

```
BEGIN PARAMETERS FOR MODEL FOAM_PLASTICITY
```

and terminates with an input line of the following form:

```
END [PARAMETERS FOR MODEL FOAM_PLASTICITY]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.

- The `thermal strain option` is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.

- Only two of the following elastic constants are required:
  - Young’s modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson’s ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.

- The initial volume fraction of solid material in the foam, $\varphi$, is defined with the `PHI` command line. For example, solid polyurethane weighs 75 pounds per cubic foot (pcf); uncompressed 10 pcf polyurethane foam would have a $\varphi$ of $0.133 = \frac{10}{75}$.

- The shear (deviatoric) strength of uncompressed foam is defined with the `SHEAR STRENGTH` command line.

- The shear hardening modulus for the foam is defined with the `SHEAR HARDENING` command line.

- The shear hardening exponent is defined with the `SHEAR EXPONENT` command line. The deviatoric strength is given by $(SHEAR STRENGTH) + (SHEAR HARDENING) \times PHI^{(SHEAR EXPONENT)}$.

- The hydrostatic (volumetric) strength of the uncompressed foam is defined with the `HYDRO STRENGTH` command line.

- The hydrodynamic hardening modulus is defined with the `HYDRO HARDENING` command line.

- The hydrodynamic hardening exponent is defined with the `HYDRO EXPONENT` command line. The hydrostatic strength is given by $(HYDRO STRENGTH) + (HYDRO HARDENING) \times PHI^{(HYDRO EXPONENT)}$.

- The prescription for nonassociated flow, $\beta$, is defined with the `BETA` command line. When $\beta = 0.0$, the flow direction is given by the normal to the yield surface (associated flow). When $\beta = 1.0$, the flow direction is given by the stress tensor. Values between 0.0 and 0.95 are recommended.
4.2.12 Elastic Three-Dimensional Orthotropic Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
BEGIN PARAMETERS FOR MODEL ELASTIC_3D_ORTHOTROPIC
  YOUNGS MODULUS AA = <real>Eaa_value
  YOUNGS MODULUS BB = <real>Ebb_value
  YOUNGS MODULUS CC = <real>Ecc_value
  POISSONS RATIO AB = <real>NUab_value
  POISSONS RATIO BC = <real>NUbc_value
  POISSONS RATIO CA = <real>NUca_value
  SHEAR MODULUS AB = <real>Gab_value
  SHEAR MODULUS BC = <real>Gbc_value
  SHEAR MODULUS CA = <real>Gca_value
  COORDINATE SYSTEM = <string>coordinate_system_name
  DIRECTION FOR ROTATION = <real>1|2|3
  ALPHA = <real>alpha_in_degrees
  SECOND DIRECTION FOR ROTATION = <real>1|2|3
  SECOND ALPHA = <real>second_alpha_in_degrees
  THERMAL STRAIN AA FUNCTION = <string>ethaa_function_name
  THERMAL STRAIN BB FUNCTION = <string>ethbb_function_name
  THERMAL STRAIN CC FUNCTION = <string>ethcc_function_name
END [PARAMETERS FOR MODEL ELASTIC_3D_ORTHOTROPIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

The elastic three-dimensional orthotropic model describes the linear elastic response of an orthotropic material where the orientation of the principal material directions can be arbitrary. These principal axes are here denoted as A, B, and C. Thermal strains are also given along the principal material axes. The specification of these material axes is accomplished by selecting a user-defined coordinate system that can then be rotated twice about one of its current axes to give the final desired directions.

For an elastic three-dimensional orthotropic model, the command block starts with the input line:

BEGIN PARAMETERS FOR MODEL ELASTIC_3D_ORTHOTROPIC

and terminates with an input line of the following form:

END [PARAMETERS FOR MODEL ELASTIC_3D_ORTHOTROPIC]

In the above command blocks:

- The density of the material is defined with the DENSITY command line.
- The Youngs moduli corresponding to the principal material axes A, B, and C are given by the YOUNGS MODULUS AA, YOUNGS MODULUS BB, and YOUNGS MODULUS CC command lines.
- The Poisson’s ratio defining the BB normal strain when the material is subjected only to AA normal stress is given by the POISSONS RATIO AB command line.
- The Poisson’s ratio defining the CC normal strain when the material is subjected only to BB normal stress is given by the \texttt{POISSONS RATIO BC} command line.

- The Poisson’s ratio defining the AA normal strain when the material is subjected only to CC normal stress is given by the \texttt{POISSONS RATIO CA} command line.

- The shear moduli for shear in the AB, BC, and CA planes are given by the \texttt{SHEAR MODULUS AB}, \texttt{SHEAR MODULUS BC}, and \texttt{SHEAR MODULUS CA} command lines, respectively.

- The specification of the principal material directions begins with the selection of a user-specified coordinate system given by the \texttt{COORDINATE SYSTEM} command line. This initial coordinate system can then be rotated twice to give the final material directions.

- The rotation of the initial coordinate system is defined using the \texttt{DIRECTION FOR ROTATION} and \texttt{ALPHA} command lines. The axis for rotation of the initial coordinate system is specified by the \texttt{DIRECTION FOR ROTATION} command line, while the angle of rotation is given by the \texttt{ALPHA} command line. This gives an intermediate specification of the material directions.

- The rotation of the intermediate coordinate system is defined using the \texttt{SECOND DIRECTION FOR ROTATION} and \texttt{SECOND ALPHA} command lines. The axis for rotation of the intermediate coordinate system is specified by the \texttt{SECOND DIRECTION FOR ROTATION} command line, while the angle of rotation is given by the \texttt{SECOND ALPHA} command line. The resulting coordinate system gives the final specification of the material directions.

- The thermal strain functions for normal thermal strains along the principal material directions are given by the \texttt{THERMAL STRAIN AA FUNCTION}, \texttt{THERMAL STRAIN BB FUNCTION}, and \texttt{THERMAL STRAIN CC FUNCTION} command lines.

See Reference 8 for more information about the elastic three-dimensional orthotropic model.
4.2.13 Orthotropic Crush Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
<string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
<string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
<string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL ORTHOTROPIC_CRUSH
YOUNGS MODULUS = <real>youngs_modulus
POISSONS RATIO = <real>poissons_ratio
SHEAR MODULUS = <real>shear_modulus
BULK MODULUS = <real>bulk_modulus
LAMBDA = <real>lambda
YIELD STRESS = <real>yield_stress
EX = <real>modulus_x
EY = <real>modulus_y
EZ = <real>modulus_z
GXY = <real>shear_modulus_xy
GYZ = <real>shear_modulus_yz
GZX = <real>shear_modulus_zx
VMIN = <real>min_crush_volume
CRUSH XX = <string>stress_volume_xx_function_name
CRUSH YY = <string>stress_volume_yy_function_name
CRUSH ZZ = <string>stress_volume_zz_function_name
CRUSH XY = <string>shear_stress_volume_xy_function_name
CRUSH YZ = <string>shear_stress_volume_yz_function_name
CRUSH ZX = <string>shear_stress_volume_zx_function_name
END [PARAMETERS FOR MODEL ORTHOTROPIC_CRUSH]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

The orthotropic crush model is an empirically based constitutive relation that is useful for modeling materials like metallic honeycomb and wood. This particular implementation follows the formulation of the metallic honeycomb model in DYNA3D [9]. The orthotropic crush model divides material behavior into three phases:

- orthotropic elastic,
- volumetric crush (partially compacted), and
- elastic–perfectly plastic (fully compacted).
4.2. MODEL SPECIFICATIONS

For an orthotropic crush material, an orthotropic crush command block starts with the input line:

```
BEGIN PARAMETERS FOR MODEL ORTHOTROPIC_CRUSH
```

and terminates with an input line of the following form:

```
END [PARAMETERS FOR MODEL ORTHOTROPIC_CRUSH]
```

In the above command blocks:

- The uncompacted density of the material is defined with the \texttt{DENSITY} command line.
- The \{thermal strain option\} is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.
- Only two of the following elastic constants are required:
  - Young’s modulus for the fully compacted state is defined with the \texttt{YOUNGS MODULUS} command line. This is the elastic–perfectly plastic value of Young’s modulus.
  - Poisson’s ratio for the fully compacted state is defined with the \texttt{POISSONS RATIO} command line. This is the elastic–perfectly plastic value of Poisson’s ratio.
  - The bulk modulus is defined with the \texttt{BULK MODULUS} command line.
  - The shear modulus is defined with the \texttt{SHEAR MODULUS} command line.
  - Lambda is defined with the \texttt{LAMBDA} command line.
- The yield stress for the fully compacted state is defined with the \texttt{YIELD STRESS} command line. This is the elastic–perfectly plastic value of the yield stress.
- The initial directional modulus $E_{xx}$ is defined with the \texttt{EX} command line.
- The initial directional modulus $E_{yy}$ is defined with the \texttt{EY} command line.
- The initial directional modulus $E_{zz}$ is defined with the \texttt{EZ} command line.
- The initial directional shear modulus $G_{xy}$ is defined with the \texttt{GXY} command line.
- The initial directional shear modulus $G_{yz}$ is defined with the \texttt{GYZ} command line.
- The initial directional shear modulus $G_{zx}$ is defined with the \texttt{GZX} command line.
- The minimum crush volume as a fraction of the original volume is defined with the \texttt{VMIN} command line.
- The directional stress $\sigma_{xx}$ as a function of the volume crush is defined by the function referenced in the \texttt{CRUSH XX} command line.
- The directional stress $\sigma_{yy}$ as a function of the volume crush is defined by the function referenced in the \texttt{CRUSH YY} command line.
- The directional stress $\sigma_{zz}$ as a function of the volume crush is defined by the function referenced in the \texttt{CRUSH ZZ} command line.
- The directional stress $\sigma_{xy}$ as a function of the volume crush is defined by the function referenced in the `CRUSH XY` command line.

- The directional stress $\sigma_{yz}$ as a function of the volume crush is defined by the function referenced in the `CRUSH YZ` command line.

- The directional stress $\sigma_{zx}$ as a function of the volume crush is defined by the function referenced in the `CRUSH ZX` command line.

Note that several of the command lines in this command block (those beginning with `CRUSH`) reference functions. These functions must be defined in the domain scope. For information about the orthotropic crush model, consult Reference 9.
4.2. MODEL SPECIFICATIONS

4.2.14 Orthotropic Rate Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
#
#{thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
  <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
  <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
  <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL ORTHOTROPIC_RATE
#
YOUNGS MODULUS = <real>youns_modulus
POISSONS RATIO = <real>poissons_ratio
SHEAR MODULUS = <real>shear_modulus
BULK MODULUS = <real>bulk_modulus
LAMBDA = <real>lambda
YIELD STRESS = <real>yield_stress
MODULUS TTTT = <real>modulus_tttt
MODULUS TTLL = <real>modulus_ttll
MODULUS TTWW = <real>modulus_ttww
MODULUS LLLL = <real>modulus_llll
MODULUS LLWW = <real>modulus_llww
MODULUS WWWW = <real>modulus_wwww
MODULUS TLTL = <real>modulus_tlrl
MODULUS LWLW = <real>modulus_lwlw
MODULUS WTWT = <real>modulus_wttt
TX = <real>tx
TY = <real>ty
TZ = <real>tz
LX = <real>lx
LY = <real>ly
LZ = <real>lz
MODULUS FUNCTION = <string>modulus_function_name
RATE FUNCTION = <string>rate_function_name
T FUNCTION = <string>t_function_name
L FUNCTION = <string>l_function_name
W FUNCTION = <string>w_function_name
TL FUNCTION = <string>tl_function_name
LW FUNCTION = <string>lw_function_name
WT FUNCTION = <string>wt_function_name
END [PARAMETERS FOR MODEL ORTHOTROPIC_RATE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
The orthotropic rate model extends the functionality of the orthotropic crush constitutive model described in Section 4.2.13. The orthotropic rate model has been developed to describe the behavior of an aluminum honeycomb subjected to large deformation. The orthotropic rate model, like the original orthotropic crush model, has six independent yield functions that evolve with volume strain. Unlike the orthotropic crush model, the orthotropic rate model has yield functions that also depend on strain rate. The orthotropic rate model also uses an orthotropic elasticity tensor with nine elastic moduli in place of the orthotropic elasticity tensor with six elastic moduli used in the orthotropic crush model. A honeycomb orientation capability is included with the orthotropic rate model that allows users to prescribe initial honeycomb orientations that are not aligned with the original global coordinate system.

For an orthotropic rate material, an orthotropic rate command block starts with the input line:

```
BEGIN PARAMETERS FOR MODEL ORTHOTROPIC_RATE
```

and terminates with an input line of the following form:

```
END [PARAMETERS FOR MODEL ORTHOTROPIC_RATE]
```

In the above command blocks:

- The density of the material is defined with the DENSITY command line.
- The \{thermal strain option\} is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.
- In the following list of elastic constants, only the elastic modulus (Young’s modulus) is required for this model. If two elastic constants are supplied, the elastic constants will be completed. However, only the elastic modulus is used in this model.
  - Young’s modulus for the fully compacted honeycomb is defined with the YOUNGS MODULUS command line.
  - Poisson’s ratio for the fully compacted state is defined with the POISSONS RATIO command line.
  - The bulk modulus for the fully compacted state is defined with the BULK MODULUS command line.
  - The shear modulus for the fully compacted state is defined with the SHEAR MODULUS command line.
  - Lambda for the fully compacted state is defined with the LAMBDA command line.
- The yield stress for the fully compacted honeycomb is defined with the YIELD STRESS command line.
- The nine elastic moduli for the orthotropic uncompacted honeycomb are defined with the MODULUS TTT, MODULUS TTTL, MODULUS TTWW, MODULUS LLLL, MODULUS LLWW, MODULUS WWW, MODULUS TLTL, MODULUS LWLW, and MODULUS WWTW command lines. The T-direction is usually associated with the generator axis for the honeycomb. The L-direction is in the ribbon plane (plane defined by flat sheets used in reinforced honeycomb) and orthogonal to the generator axis. The W-direction is perpendicular to the ribbon plane.
- The components of a vector defining the T-direction of the honeycomb are defined by the \( TX, TY, \) and \( TZ \) command lines. The values of \( tx, ty, \) and \( tz \) are components of a vector in the global coordinate system that define the orientation of the honeycomb’s T-direction (generator axis).

- The components of a vector defining the L-direction of the honeycomb are defined by the \( LX, LY, \) and \( LZ \) command lines. The values of \( lx, ly, \) and \( lz \) are components of a vector in the global coordinate system that define the orientation of the honeycomb’s L-direction. *Caution*: The vectors T and L must be orthogonal.

- The function describing the variation in moduli with compaction is given by the \texttt{MODULUS FUNCTION} command line. The moduli vary continuously from their initial orthotropic values to isotropic values when full compaction is obtained.

- The function describing the change in strength with strain rate is given by the \texttt{RATE FUNCTION} command line. Note that all strengths are scaled with the multiplier obtained from this function.

- The function describing the T-normal strength of the honeycomb as a function of compaction is given by the \texttt{T FUNCTION} command line.

- The function describing the L-normal strength of the honeycomb as a function of compaction is given by the \texttt{L FUNCTION} command line.

- The function describing the W-normal strength of the honeycomb as a function of compaction is given by the \texttt{W FUNCTION} command line.

- The function describing the TL-normal strength of the honeycomb as a function of compaction is given by the \texttt{TL FUNCTION} command line.

- The function describing the LW-normal strength of the honeycomb as a function of compaction is given by the \texttt{LW FUNCTION} command line.

- The function describing the WT-normal strength of the honeycomb as a function of compaction is given by the \texttt{WT FUNCTION} command line.

Note that several of the command lines in this command block reference functions. These functions must be defined in the domain scope.
4.2.15 Elastic Laminate Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
BEGIN PARAMETERS FOR MODEL ELASTIC_LAMINATE
A11 = <real>a11_value
A12 = <real>a12_value
A16 = <real>a16_value
A22 = <real>a22_value
A26 = <real>a26_value
A66 = <real>a66_value
A44 = <real>a44_value
A45 = <real>a45_value
A55 = <real>a55_value
B11 = <real>b11_value
B12 = <real>b12_value
B16 = <real>b16_value
B22 = <real>b22_value
B26 = <real>b26_value
B66 = <real>b66_value
D11 = <real>d11_value
D12 = <real>d12_value
D16 = <real>d16_value
D22 = <real>d22_value
D26 = <real>d26_value
D66 = <real>d66_value
COORDINATE SYSTEM = <string>coord_sys_name
DIRECTION FOR ROTATION = 1|2|3
ALPHA = <real>alpha_value_in_degrees
THETA = <real>theta_value_in_degrees
NTH11 FUNCTION = <string>nth11_function_name
NTH22 FUNCTION = <string>nth22_function_name
NTH12 FUNCTION = <string>nth12_function_name
MTH11 FUNCTION = <string>mth11_function_name
MTH22 FUNCTION = <string>mth22_function_name
MTH12 FUNCTION = <string>mth12_function_name
END [PARAMETERS FOR MODEL ELASTIC_LAMINATE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

The elastic laminate model can be used to describe the overall linear elastic response of layered shells. The response of each layer is pre-integrated through the thickness under an assumed variation of strain through the thickness. That is, the user inputs laminate stiffness matrices directly, and the overall response is calculated appropriately. This model allows the user to input laminate stiffness matrices that are consistent with a state of generalized plane stress for each layer. Each layer can be orthotropic with a unique orientation. This model is primarily intended for capturing the response of fiber-reinforced laminated composites. The user inputs the laminate stiffness
matrices calculated with respect to a chosen coordinate system and then specifies this coordinate system’s definition relative to the global coordinate system. Thermal stresses are handled via the input of thermal-force and thermal-force-couple resultants for the laminate as a whole. At present, the user cannot get layer stresses out from this material model. However, the overall section-force and force-couple resultants can be computed from available output. The details of this model are described in References 10 and 11.

For elastic laminate materials, the elastic laminate command block begins with the input line:

```
BEGIN PARAMETERS FOR MODEL ELASTIC_LAMINATE
```

and terminates with an input line of the following form:

```
END [PARAMETERS FOR MODEL ELASTIC_LAMINATE]
```

In the above command blocks:

- The density of the material is defined with the `DENSITY` command line.
- The extensional stiffnesses are defined with the \( A_{ij} \) command lines, where the values of \( i,j \) are 11, 12, 16, 22, 26, 66, 44, 45, and 55.
- The coupling stiffnesses are defined with the \( B_{ij} \) command lines, where the values of \( i,j \) are 11, 12, 16, 22, 26, and 66.
- The bending stiffnesses are defined with the \( D_{ij} \) command lines, where the values of \( i,j \) are 11, 12, 16, 22, 26, and 66.
- The initial laminate coordinate system is defined with the `COORDINATE SYSTEM` command line.
- The rotation of the initial laminate coordinate system is defined with the `DIRECTION FOR ROTATION` and `ALPHA` command lines. The axis of initial laminate coordinate system is specified by the `DIRECTION FOR ROTATION` command line, while the angle of rotation is given by the `ALPHA` command line. This produces an intermediate laminate coordinate system that is then projected onto the surface of each shell element.
- The projected intermediate laminate coordinate system is rotated about the element normal by angle theta, which is specified by the `THETA` command line.
- The thermal-force resultants are defined by functions that are referenced on the `NTH11 FUNCTION`, `NTH22 FUNCTION`, and `NTH12 FUNCTION` command lines.
- The thermal-force-couple resultants are defined by functions that are referenced on the `MTH11 FUNCTION`, `MTH22 FUNCTION`, and `MTH12 FUNCTION` command lines.
4.2.16 Fiber Membrane Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
<string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
<string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
<string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL FIBER_MEMBRANE
YOUNGS MODULUS = <real>younsgs_modulus
POISSONS RATIO = <real>poissons_ratio
SHEAR MODULUS = <real>shear_modulus
BULK MODULUS = <real>bulf_modulus
LAMBDA = <real>lambda
CORD DENSITY = <real>cord_density
CORD DIAMETER = <real>cord_diameter
MATRIX DENSITY = <real>matrix_density
TENSILE TEST FUNCTION = <string>test_function_name
PERCENT CONTINUUM = <real>percent_continuum
EPL = <real>epl
AXIS X = <real>axis_x
AXIS Y = <real>axis_y
AXIS Z = <real>axis_z
MODEL = <string>RECTANGULAR
STIFFNESS SCALE = <real>stiffness_scale
REFERENCE STRAIN = <real>reference_strain
END [PARAMETERS FOR MODEL FIBER_MEMBRANE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

The fiber membrane model is used for modeling membranes that are reinforced with unidirectional fibers. Through the use of a non-zero PERCENT CONTINUUM, a background isotropic material response can also be incorporated and is added in a manner such that the response in the fiber direction is unchanged. The fiber membrane model can be used in both Presto and Adagio. When the fiber membrane model is used in Adagio, the model can be used with or without the control-stiffness option in Adagio’s multilevel solver. The control-stiffness option is implemented via the CONTROL STIFFNESS command block and is discussed in Chapter 3 of the Adagio user’s guide. If the control-stiffness option is activated in Adagio, the response in the fiber direction is softened by lowering the fiber response. In all cases, the final material behavior that is used for equilibrium corresponds to the real material response. When the fiber membrane model is used in Presto, the fiber scaling, which is controlled by the STIFFNESS SCALE command line, is ignored.
4.2. MODEL SPECIFICATIONS

For a fiber membrane material, a fiber membrane command block starts with the input line:

BEGIN PARAMETERS FOR MODEL FIBER_MEMBRANE

and terminates with an input line of the following form:

END [PARAMETERS FOR MODEL FIBER_MEMBRANE]

In the above command blocks, the following definitions are applicable. Usage requirements are identified both in this list of definitions and in the discussion that follows the list.

- The density of the material is defined with the DENSITY command line. This command line should be included, but its value will be recomputed (and hence replaced) if the CORD DENSITY, CORD DIAMETER, and MATRIX DENSITY command lines are specified.

- The \{thermal strain option\} is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.

- Only two of the following elastic constants are required. These are used to compute values for the elastic preconditioner only.
  
  - Young’s modulus is defined with the YOUNGS MODULUS command line.
  
  - Poisson’s ratio is defined with the POISSONS RATIO command line.
  
  - The bulk modulus is defined with the BULK MODULUS command line.
  
  - The shear modulus is defined with the SHEAR MODULUS command line.
  
  - Lambda is defined with the LAMBDA command line.

- The density of the bers is defined by the CORD DENSITY command line. This command line is optional. See the usage discussion below.

- The diameter of the bers is defined by the CORD DIAMETER command line. This command line is optional. See the usage discussion below.

- The density of the matrix is defined by the MATRIX DENSITY command line. This command line is optional. See the usage discussion below.

- The tensile test function command line references the name of a function defined in a DEFINITION FOR FUNCTION command line in the domain scope that describes the fiber force versus strain data. This command line must be included.

- The fractional bers stiffness to use in defining the background isotropic response is given by the PERCENT CONTINUUM command line. This command line must be included.

- The number of bers per unit length is defined by the EPL command line. This command line must be included.

- The components of the vector defining the initial bers direction is given by the AXIS X, AXIS Y, and AXIS Z command lines. These command lines must be included. See the usage discussion below.
- The coordinate system for specifying the fiber orientation is given by the `MODEL` command line. Only the option `RECTANGULAR` is available in this release. This command line must be included. See the usage discussion below.

- The fiber scaling is specified by the `STIFFNESS SCALE` command line. If the control-stiffness option is used in Adagio, this command line must be included. When the fiber membrane model is used in Presto, this command line is ignored.

- The reference strain is defined with the `REFERENCE STRAIN` command line. This command line is optional for Adagio and is not used in Presto. If the control-stiffness option is used in Adagio, this command line may be included. See the usage discussion below.

Certain command lines in the `PARAMETERS FOR MODEL FIBER_MEMBRANE` command block also have interdependencies or other factors that may impact their usage in Presto and Adagio, as discussed below.

The `CORD DENSITY`, `CORD DIAMETER`, and `MATRIX DENSITY` command lines are optional. When included, these three command lines are used for computation of the correct density corresponding to the fibers, the number of fibers per unit length, and the chosen matrix. When these three command lines are not included, the density is taken as that specified by the `DENSITY` command line.

The `AXIS X`, `AXIS Y`, and `AXIS Z` command lines must be specified if the value for the `MODEL` command line is `RECTANGULAR`. Currently, these axis-related command lines must be specified.

Specifying a reference strain (via the `REFERENCE STRAIN` command line) implies the use of strains for measuring part of the control-stiffness material constraint violation in Adagio. If this command line is not present, the material constraint violation is determined by comparing the change in the scaled fiber force over the current model problem.
### 4.2.17 Incompressible Solid Model

```plaintext
BEGIN PROPERTY SPECIFICATION FOR MATERIAL "mat_name"
  DENSITY = <real>density_value
  
  # {thermal strain option}
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function

BEGIN PARAMETERS FOR MODEL INCOMPRESSIBLE SOLID
  YOUNGS MODULUS = <real>youngs_modulus
  POISSONS RATIO = <real>poissons_ratio
  BULK MODULUS = <real>bulk_modulus
  SHEAR MODULUS = <real>shear_modulus
  LAMBDA = <real>lambda
  K SCALING = <real>k_scaling
  2G SCALING = <real>2g_scaling
  TARGET E = <real>target_e
  MAX POISSONS RATIO = <real>max_poissons_ratio
  REFERENCE STRAIN = <real>reference_strain
  SCALING FUNCTION = <string>scaling_function_name
END [PARAMETERS FOR MODEL INCOMPRESSIBLE SOLID]
END [PROPERTY SPECIFICATION FOR MATERIAL "mat_name"]
```

The incompressible solid model is a variation of the elastic model and can be used in both Presto and Adagio. In Adagio, the incompressible solid model is used with the control-stiffness option in the multilevel solver. The control-stiffness option is implemented via the `CONTROL STIFFNESS` command block and is discussed in Chapter 3 of the Adagio user’s guide. The model is used to model nearly incompressible materials where Poisson’s ratio, $\nu$, $\approx 0.5$. In the course of solving a series of model problems in Adagio, the material response from this model incorporates scaling the bulk and/or shear behaviors to yield a material response that is more amenable to solution using Adagio’s conjugate gradient solver. The final material behavior that is calculated corresponds to the actual moduli that are specified. When this model is used in Presto, the material scalings are ignored, and the model behaves like a linear elastic model.

For an incompressible solid material, an incompressible solid command block starts with the input line:

```plaintext
BEGIN PARAMETERS FOR MODEL INCOMPRESSIBLE SOLID
```

and terminates with an input line of the following form:

```plaintext
END [PARAMETERS FOR MODEL INCOMPRESSIBLE SOLID]
```
In the above command blocks, the following definitions are applicable. Usage requirements are identified both in this list of definitions and in the discussion that follows the list.

- The density of the material is defined with the `DENSITY` command line.

- The `{thermal strain option}` is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.

- Only two of the following elastic constants are required to define the unscaled material response:
  
  - Young’s modulus is defined with the `YOUNGS MODULUS` command line.
  - Poisson’s ratio is defined with the `POISSONS RATIO` command line.
  - The bulk modulus is defined with the `BULK MODULUS` command line.
  - The shear modulus is defined with the `SHEAR MODULUS` command line.
  - Lambda is defined with the `LAMBDA` command line.

- The following material-scaling command lines are used only in Adagio:
  
  - The nominal bulk scaling is defined with the `K SCALING` command line. This command line is optional. See the usage discussion below.
  - The nominal shear scaling is defined with the `2G SCALING` command line. This command line is optional. See the usage discussion below.
  - The target Young’s modulus is defined with the `TARGET E` command line. This command line is optional. See the usage discussion below.
  - The maximum Poisson’s ratio is defined with the `MAX POISSONS RATIO` command line. This command line is optional. See the usage discussion below.
  - The reference strain is defined with the `REFERENCE STRAIN` command line. This command line is optional. See the usage discussion below.
  - The `SCALING FUNCTION` command line references the name of a function defined in a `DEFINITION FOR FUNCTION` command line in the domain scope that describes the time dependent scaling to be applied. This command line is optional. See the usage discussion below.

As noted previously, only two of the elastic constants are required to define the unscaled material response. This requirement applies to use of the incompressible solid model in Presto and in Adagio. Further, all the material-scaling command lines are only used in Adagio.

Several options exist for defining the bulk and/or shear scalings that can be used with the multilevel solver in Adagio.
- Option 1: You can provide the scalings directly by including both of the K SCALING and 2G SCALING command lines or either of them. When both command lines are input, the user-specified values for their parameters will be used. If only the K SCALING command line is input, the bulk scaling is as specified in the k_scaling parameter, and the value of the shear scaling parameter, 2g_scaling, is set to 1.0. On the other hand, if only the 2G SCALING command line is input, then the shear scaling is as specified in the 2g_scaling parameter, but the value of the bulk-scaling parameter, k_scaling, is not set to 1.0. Instead, the bulk scaling is determined by computing a scaled bulk modulus from the scaled shear modulus and a (scaled) Poisson’s ratio of 0.3. Then, the bulk scaling is determined simply as the ratio of the scaled bulk modulus to the actual bulk modulus.

- Option 2: You can specify either or both of the TARGET E and MAX POISSONS RATIO command lines to define the scalings. If only the TARGET E command line is included, the bulk and shear scalings are computed by first finding scaled moduli using the value of the target_e parameter along with a (scaled) Poisson’s ratio of 0.3. The bulk and shear scalings are then determined as the ratio of the appropriate scaled to unscaled modulus. If only the MAX POISSONS RATIO command line is included, the shear scaling is set to 1.0, and the bulk scaling is computed by first calculating a scaled bulk modulus from the actual shear modulus and the value of the max_poissons_ratio parameter. The bulk scaling is then calculated simply as the ratio of the scaled bulk modulus to the actual bulk modulus. If both the TARGET E and MAX POISSONS RATIO command lines are included, the bulk scaling (and shear scaling) is determined from the ratio of the bulk scaled modulus (and shear scaled modulus) computed using the values of the target_e and max_poissons_ratio parameters to the unscaled bulk (and shear) modulus.

- Option 3: You can choose not to include any of the K SCALING, 2G SCALING, TARGET E, and MAX POISSONS RATIO command lines. In such case, the shear scaling is set to 1.0, and the bulk scaling is computed as the ratio of the scaled bulk modulus coming from the real shear modulus and a (scaled) Poisson’s ratio of 0.3 to the actual bulk modulus.

The function referenced by the value of the parameter scaling_function_name in the SCALING FUNCTION command line can be used to modify the bulk and shear scalings in solution time. The actual scalings used are computed by taking the scalings specified by the parameter values in the K SCALING, 2G SCALING, TARGET E, and MAX POISSONS RATIO command lines and simply multiplying them by the function value at the specified solution time. If the SCALING FUNCTION command line is not included, the bulk and shear scalings are fixed in time.

The REFERENCE STRAIN command line supplies a value for the reference strain that is used to create a normalized material constraint violation based on strains. Specifying a reference strain implies the use of strains for measuring the material constraint violation (or part of the control-stiffness error in Adagio). Otherwise, the material constraint violation is determined by using the change in the scaled stress response over the current model problem.
4.2.18  Mooney-Rivlin Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
#
BEGIN PARAMETERS FOR MODEL MOONEY_RIVLIN
  YOUNGS MODULUS = <real>youngs_modulus
  POISSONS RATIO = <real>poissons_ratio
  BULK MODULUS = <real>bulk_modulus
  SHEAR MODULUS = <real>shear_modulus
  LAMBDA = <real>lambda
  C10 = <real>c10
  C01 = <real>c01
  C10 FUNCTION = <string>c10_function_name
  C01 FUNCTION = <string>c01_function_name
  BULK FUNCTION = <string>bulk_function_name
  THERMAL EXPANSION FUNCTION = <string>eth_function_name
  TARGET E = <real>target_e
  TARGET E FUNCTION = <string>etar_function_name
  MAX POISSONS RATIO = <real>max_poissons_ratio
  REFERENCE STRAIN = <real>reference_strain
END [PARAMETERS FOR MODEL MOONEY_RIVLIN]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

Mooney-Rivlin is a hyperelastic model that is used to model rubber. The Mooney-Rivlin model incorporates temperature-dependent material moduli and can be used in both Presto and Adagio. When the model is used in Adagio, it can be used with or without the control-stiffness option in Adagio’s multilevel solver. The control-stiffness option is implemented via the CONTROL STIFFNESS command block and is discussed in Chapter 3 of the Adagio user’s guide. The model is used to model nearly incompressible materials where Poisson’s ratio, \( \nu \), \( \approx 0.5 \). In the course of solving a series of model problems in Adagio, the material response from this model incorporates scaling the bulk and/or shear behaviors to yield a material response that is more amenable to solution using Adagio’s conjugate gradient solver. The final material behavior that is calculated corresponds to the actual moduli that are specified. When this model is used in Presto, the material scalings are ignored.

For a Mooney-Rivlin material, a Mooney-Rivlin command block starts with the input line:

BEGIN PARAMETERS FOR MODEL MOONEY_RIVLIN

and terminates an input line of the following form:

END [PARAMETERS FOR MODEL MOONEY_RIVLIN]

In the above command blocks:

- The density of the material is defined with the DENSITY command line.
- Only two of the following elastic constants are required to define the unscaled bulk behavior:
• Young’s modulus is defined with the YOUNGS MODULUS command line.
• Poisson’s ratio is defined with the POISSONS RATIO command line.
• The bulk modulus is defined with the BULK MODULUS command line.
• The shear modulus is defined with the SHEAR MODULUS command line.
• Lambda is defined with the LAMBDA command line.

- The nominal value for C10 is defined with the c10 command line. This command line is required. See the usage discussion below.

- The nominal value for C01 is defined with the c01 command line. This command line is required. See the usage discussion below.

- The C10 FUNCTION command line references the name of a function defined in a DEFINITION FOR FUNCTION command line in the domain scope that describes the temperature dependence of the C10 material parameter. This command line is optional. See the usage discussion below.

- The C01 FUNCTION command line references the name of a function defined in a DEFINITION FOR FUNCTION command line in the domain scope that describes the temperature dependence of the C01 material parameter. This command line is optional. See the usage discussion below.

- The BULK FUNCTION command line references the name of a function defined in a DEFINITION FOR FUNCTION command line in the domain scope that describes the temperature dependence of the bulk modulus. This command line is optional. See the usage discussion below.

- The THERMAL EXPANSION FUNCTION command line references the name of a function defined in a DEFINITION FOR FUNCTION command line in the domain scope that describes the linear thermal expansion as function of temperature. This command line is optional. See the usage discussion below.

- The following material-scaling command lines are used only in Adagio:

  • The target Young’s modulus is defined with the TARGET E command line. This command line is optional. See the usage discussion below.

  • The TARGET E FUNCTION command line references the name of a function defined in a DEFINITION FOR FUNCTION command line in the domain scope that describes the time variation of the target Young’s modulus. This command line is optional. See the usage discussion below.

  • The maximum Poisson’s ratio is defined with the MAX POISSONS RATIO command line. This command line is optional. See the usage discussion below.

  • The reference strain is defined with the REFERENCE STRAIN command line. This command line is optional. See the usage discussion below.
As noted previously, only two of the elastic constants are required to define the unscaled bulk behavior. Together, the values for C10 and C01 determine the shear behavior, and thus the C10 and C01 command lines must be included in this model.

The command lines for functions that specify the temperature dependence of C10, C01, and bulk modulus are optional, e.g., the C10 FUNCTION, C01 FUNCTION and BULK FUNCTION command lines. If these command lines are not included, their corresponding material parameters are taken to be independent of temperature. Mooney-Rivlin, like other material models, allows for the specification of thermal strain behavior within the material model itself, via the THERMAL EXPANSION FUNCTION command line. This command line, like the other “function-type” command lines in this model requires that a function associated with the name be defined in the domain scope.

The bulk and shear scalings that can be used with the multilevel solver in Adagio are specified via a combination of the TARGET E, TARGET E FUNCTION, and MAX POISSONS RATIO command lines. If the TARGET E command line is not included (and the MAX POISSONS RATIO command line is included), the shear scaling is set to 1.0, and the bulk scaling is determined from the ratio of the scaled bulk modulus to its unscaled value, where the scaled bulk modulus is computed using the value of the max_poissons_ratio parameter along with the unscaled initial shear modulus that is determined from the value of the parameters specified in the C10 and C01 command lines. On the other hand, if both the TARGET E command line and the MAX POISSONS RATIO command line are included, bulk and shear scaling values are computed using scaled moduli that are calculated from the target_e and max_poissons_ratio parameter values.

Including the TARGET E FUNCTION command line allows time-dependent bulk and shear scaling to be used. If this command line is not specified, the bulk and shear scalings remain constant in solution time. If the command line is specified, the target Young’s modulus that is used for computing the scaled moduli is multiplied by the function value.

The REFERENCE STRAIN command line supplies a value for the reference strain used to create a normalized material constraint violation that is based on strains. Specifying a reference strain implies the use of strains for measuring the material constraint violation (or part of the control-stiffness error in Adagio). Otherwise, the material constraint violation is determined using the change in the scaled stress response over the current model problem.

Brief documentation on the theoretical basis for the Mooney-Rivlin model is given in Reference 12.
4.2.19 NLVE 3D Orthotropic Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
#
BEGIN PARAMETERS FOR MODEL NLVE_3D_ORTHOTROPIC
  YOUNGS MODULUS = <real>younsgs_modulus
  POISSONS RATIO = <real>poissons_ratio
  SHEAR MODULUS = <real>shear_modulus
  BULK MODULUS = <real>bulk_modulus
  LAMBDA = <real>lambda
  COORDINATE SYSTEM = <string>coordinate_system_name
  DIRECTION FOR ROTATION = <real>1|2|3
  ALPHA = <real>alpha_in_degrees
  SECOND DIRECTION FOR ROTATION = <real>1|2|3
  SECOND ALPHA = <real>second_alpha_in_degrees
  FICTITIOUS LOGA FUNCTION = <string>fict_loga_function_name
  FICTITIOUS LOGA SCALE FACTOR = <real>fict_loga_scale_factor
#
# In each of the five ‘PRONY’ command lines and in
# the RELAX TIME command line, the value of i can be from
# 1 through 30
  1PSI PRONY <integer>i = <real>psi1_i
  2PSI PRONY <integer>i = <real>psi2_i
  3PSI PRONY <integer>i = <real>psi3_i
  4PSI PRONY <integer>i = <real>psi4_i
  5PSI PRONY <integer>i = <real>psi5_i
  RELAX TIME <integer>i = <real>tau_i
  REFERENCE TEMP = <real>tref
  REFERENCE DENSITY = <real>rhoref
  WLF C1 = <real>wlf_c1
  WLF C2 = <real>wlf_c2
  B SHIFT CONSTANT = <real>b_shift
  SHIFT REF VALUE = <real>shift_ref
  WWBETA 1PSI = <real>wwb_1psi
  WWTAU 1PSI = <real>wwt_1psi
  WWBETA 2PSI = <real>wwb_2psi
  WWTAU 2PSI = <real>wwt_2psi
  WWBETA 3PSI = <real>wwb_3psi
  WWTAU 3PSI = <real>wwt_3psi
  WWBETA 4PSI = <real>wwb_4psi
  WWTAU 4PSI = <real>wwt_4psi
  WWBETA 5PSI = <real>wwb_5psi
  WWTAU 5PSI = <real>wwt_5psi
  DOUBLE INTEG FACTOR = <real>dble_int_fac
  REF RUBBERY HCAPACITY = <real>hcapr
  REF GLASSY HCAPACITY = <real>hcapg
  GLASS TRANSITION TEM = <real>tg
REF GLASSY C11 = <real>c11g
REF RUBBERY C11 = <real>c11r
REF GLASSY C22 = <real>c22g
REF RUBBERY C22 = <real>c22r
REF GLASSY C33 = <real>c33g
REF RUBBERY C33 = <real>c33r
REF GLASSY C12 = <real>c12g
REF RUBBERY C12 = <real>c12r
REF GLASSY C13 = <real>c13g
REF RUBBERY C13 = <real>c13r
REF GLASSY C23 = <real>c23g
REF RUBBERY C23 = <real>c23r
REF GLASSY C44 = <real>c44g
REF RUBBERY C44 = <real>c44r
REF GLASSY C55 = <real>c55g
REF RUBBERY C55 = <real>c55r
REF GLASSY C66 = <real>c66g
REF RUBBERY C66 = <real>c66r
REF GLASSY CTE1 = <real>cte1g
REF RUBBERY CTE1 = <real>cte1r
REF GLASSY CTE2 = <real>cte2g
REF RUBBERY CTE2 = <real>cte2r
REF GLASSY CTE3 = <real>cte3g
REF RUBBERY CTE3 = <real>cte3r
LINEAR VISCO TEST = <real>lvt
T DERIV GLASSY C11 = <real>dc11gdT
T DERIV RUBBERY C11 = <real>dc11rdT
T DERIV GLASSY C22 = <real>dc22gdT
T DERIV RUBBERY C22 = <real>dc22rdT
T DERIV GLASSY C33 = <real>dc33gdT
T DERIV RUBBERY C33 = <real>dc33rdT
T DERIV GLASSY C12 = <real>dc12gdT
T DERIV RUBBERY C12 = <real>dc12rdT
T DERIV GLASSY C13 = <real>dc13gdT
T DERIV RUBBERY C13 = <real>dc13rdT
T DERIV GLASSY C23 = <real>dc23gdT
T DERIV RUBBERY C23 = <real>dc23rdT
T DERIV GLASSY C44 = <real>dc44gdT
T DERIV RUBBERY C44 = <real>dc44rdT
T DERIV GLASSY C55 = <real>dc55gdT
T DERIV RUBBERY C55 = <real>dc55rdT
T DERIV GLASSY C66 = <real>dc66gdT
T DERIV RUBBERY C66 = <real>dc66rdT
T DERIV GLASSY CTE1 = <real>dcte1gdT
T DERIV RUBBERY CTE1 = <real>dcte1rdT
T DERIV GLASSY CTE2 = <real>dcte2gdT
T DERIV RUBBERY CTE2 = <real>dcte2rdT
4.2. MODEL SPECIFICATIONS

T DERIV GLASSY CTE3 = <real>dcte3dT
T DERIV RUBBERY CTE3 = <real>dcte3rdT
T DERIV GLASSY HCAPACITY = <real>dhcapgdT
T DERIV RUBBERY HCAPACITY = <real>dhcaprdT
REF PSIC = <real>psic_ref
T DERIV PSIC = <real>dpsicdT
T 2DERIV PSIC = <real>d2psicdT2
PSI EQ 2T = <real>psitt
PSI EQ 3T = <real>psittt
PSI EQ 4T = <real>psitttt
PSI EQ XX 11 = <real>psiXX11
PSI EQ XX 22 = <real>psiXX22
PSI EQ XX 33 = <real>psiXX33
PSI EQ XX 12 = <real>psiXX12
PSI EQ XX 13 = <real>psiXX13
PSI EQ XX 23 = <real>psiXX23
PSI EQ XX 44 = <real>psiXX44
PSI EQ XX 55 = <real>psiXX55
PSI EQ XX 66 = <real>psiXX66
PSI EQ XXT 11 = <real>psiXXT11
PSI EQ XXT 22 = <real>psiXXT22
PSI EQ XXT 33 = <real>psiXXT33
PSI EQ XXT 12 = <real>psiXXT12
PSI EQ XXT 13 = <real>psiXXT13
PSI EQ XXT 23 = <real>psiXXT23
PSI EQ XXT 44 = <real>psiXXT44
PSI EQ XXT 55 = <real>psiXXT55
PSI EQ XXT 66 = <real>psiXXT66
PSI EQ XT 1 = <real>psiXT1
PSI EQ XT 2 = <real>psiXT2
PSI EQ XT 3 = <real>psiXT3
PSI EQ XTT 1 = <real>psiXTT1
PSI EQ XTT 2 = <real>psiXTT2
PSI EQ XTT 3 = <real>psiXTT3
REF PSIA 11 = <real>psiA11
REF PSIA 22 = <real>psiA22
REF PSIA 33 = <real>psiA33
REF PSIA 12 = <real>psiA12
REF PSIA 13 = <real>psiA13
REF PSIA 23 = <real>psiA23
REF PSIA 44 = <real>psiA44
REF PSIA 55 = <real>psiA55
REF PSIA 66 = <real>psiA66
T DERIV PSIA 11 = <real>dpsiA11dT
T DERIV PSIA 22 = <real>dpsiA22dT
T DERIV PSIA 33 = <real>dpsiA33dT
T DERIV PSIA 12 = <real>dpsiA12dT
The NLVE three-dimensional orthotropic model is a nonlinear viscoelastic orthotropic continuum model that describes the behavior of fiber-reinforced polymer-matrix composites. In addition to being able to model the linear elastic and linear viscoelastic behaviors of such composites, it also can capture both “weak” and “strong” nonlinear viscoelastic effects such as stress dependence of the creep compliance and viscoelastic yielding. This model can be used in both Presto and Adagio. Because the NLVE model is still under active development and also because it has an extensive list of command lines, we have not followed the typical approach in documenting this model.
4.2. MODEL SPECIFICATIONS

4.2.20 Stiff Elastic

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  # {thermal strain option}
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL STIFF_ELASTIC
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    BULK MODULUS = <real>bulk_modulus
    SHEAR MODULUS = <real>shear_modulus
    LAMBDA = <real>lambda
    SCALE FACTOR = <real>scale_factor
    REFERENCE STRAIN = <real>reference_strain
  END [PARAMETERS FOR MODEL STIFF_ELASTIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

The stiff elastic model is a variation of the isotropic elastic model. The stiff elastic model can be used in both Presto and Adagio. When the model is used in Adagio, it is typically used with the control-stiffness option in Adagio’s multilevel solver. The control-stiffness option is implemented via the CONTROL STIFFNESS command block and is discussed in Chapter 3 of the Adagio user’s guide. The stiff elastic model is used to lower the stiffness of the bulk and shear behaviors of relatively stiff materials to yield a material response more amenable to solution using Adagio’s conjugate gradient solver. The final material behavior that is calculated corresponds to the actual moduli that are specified. When this model is used in Presto, the material scalings are ignored.

For a stiff elastic material, a stiff elastic command block starts with the input line:

    BEGIN PARAMETERS FOR MODEL STIFF_ELASTIC

and terminates with an input line of the following form:

    END [PARAMETERS FOR MODEL STIFF_ELASTIC]

In the above command blocks:

- The density of the material is defined with the DENSITY command line.

- The {thermal strain option} is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.
Only two of the following elastic constants are required to define the unscaled material response:

- Young’s modulus is defined with the YOUNGS MODULUS command line.
- Poisson’s ratio is defined with the POISSONS RATIO command line.
- The bulk modulus is defined with the BULK MODULUS command line.
- The shear modulus is defined with the SHEAR MODULUS command line.
- Lambda is defined with the LAMBDA command line.

The following command lines are used only in Adagio:

- The material scaling is defined with the SCALE FACTOR command line.
- The reference strain is defined with the REFERENCE STRAIN command line.

As noted previously, only two of the elastic constants are required to define the unscaled material response.

The scaled bulk and shear moduli are computed using a Young’s modulus scaled by the value given by the SCALE FACTOR line command.

The REFERENCE STRAIN command line supplies a value for the reference strain used to create a normalized material constraint violation that is based on strains. Specifying a reference strain implies the use of strains for measuring the material constraint violation (or part of the control-stiffness error in Adagio). Otherwise, the material constraint violation is determined using the change in the scaled stress response over the current model problem.
4.2.21 Swanson Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
   DENSITY = <real>density_value
#
BEGIN PARAMETERS FOR MODEL SWANSON
   YOUNGS MODULUS = <real>youngs_modulus
   POISSONS RATIO = <real>poissons_ratio
   BULK MODULUS = <real>bulk_modulus
   SHEAR MODULUS = <real>shear_modulus
   LAMBDA = <real>lambda
   A1 = <real>a1
   P1 = <real>p1
   B1 = <real>b1
   Q1 = <real>q1
   C1 = <real>c1
   R1 = <real>r1
   CUT OFF STRAIN = <real>ecut
   THERMAL EXPANSION FUNCTION = <string>eth_function_name
   TARGET E = <real>target_e
   TARGET E FUNCTION = <string>etar_function_name
   MAX POISSONS RATIO = <real>max_poissons_ratio
   REFERENCE STRAIN = <real>reference_strain
END [PARAMETERS FOR MODEL SWANSON]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

The Swanson model is a hyperelastic model that is used to model rubber. The Swanson model can be used in both Presto and Adagio. When the model is used in Adagio, it can be used with or without the control-stiffness option in Adagio’s multilevel solver for nearly incompressible materials where Poisson’s ratio, $\nu$, $\approx 0.5$. The control-stiffness option is implemented via the CONTROL STIFFNESS command block and is discussed in Chapter 3 of the Adagio user’s guide. In the course of solving a series of model problems in Adagio, the material response from this model incorporates scaling the bulk and/or shear behaviors to yield a material response that is more amenable to solution using Adagio’s conjugate gradient solver. The final material behavior that is calculated corresponds to the actual moduli that are specified. When this model is used in Presto, the material scalings are ignored.

For a Swanson material, a Swanson command block starts with the input line:

   BEGIN PARAMETERS FOR MODEL SWANSON

and terminates an input line of the following form:

   END [PARAMETERS FOR MODEL SWANSON]

In the above command blocks:

- The density of the material is defined with the DENSITY command line.
- Only two of the following elastic constants are required to define the unscaled bulk behavior:
• Young’s modulus is defined with the \texttt{YOUNGS MODULUS} command line.
• Poisson’s ratio is defined with the \texttt{POISSONS RATIO} command line.
• The bulk modulus is defined with the \texttt{BULK MODULUS} command line.
• The shear modulus is defined with the \texttt{SHEAR MODULUS} command line.
• Lambda is defined with the \texttt{LAMBDA} command line.

- The following command lines are required:
  • The material constant A1 is defined with the \texttt{A1} command line.
  • The material constant P1 is defined with the \texttt{P1} command line.
  • The material constant B1 is defined with the \texttt{B1} command line.
  • The material constant Q1 is defined with the \texttt{Q1} command line.
  • The material constant C1 is defined with the \texttt{C1} command line.
  • The material constant R1 is defined with the \texttt{R1} command line.
  • The small-strain value used for computing the initial shear modulus is defined with the \texttt{CUT OFF STRAIN} command line.

- The \texttt{THERMAL EXPANSION FUNCTION} command line references the name of a function defined in a \texttt{DEFINITION FOR FUNCTION} command line in the domain scope that describes the linear thermal expansion as function of temperature. This command line is optional. See the usage discussion below.

- The following material-scaling command lines are used only in Adagio:
  • The target Young’s modulus is defined with the \texttt{TARGET E} command line. This command line is optional. See the usage discussion below.
  • The \texttt{TARGET E FUNCTION} command line references the name of a function defined in a \texttt{DEFINITION FOR FUNCTION} command line in the domain scope that describes the time variation of the target Young’s modulus. This command line is optional. See the usage discussion below.
  • The maximum Poisson’s ratio is defined with the \texttt{MAX POISSONS RATIO} command line. This command line is optional. See the usage discussion below.
  • The reference strain is defined with the \texttt{REFERENCE STRAIN} command line. This command line is optional. See the usage discussion below.

As noted previously, only two of the elastic constants are required to define the unscaled bulk behavior. Together, the values for parameters in the A1, P1, B1, Q1, C1, and R1 command lines define the unscaled shear behavior, so these command lines must be present. The initial unscaled shear modulus is determined from those parameter values along with the value of the parameter in the \texttt{CUT OFF STRAIN} command line, so this command line must also be present.
4.2. MODEL SPECIFICATIONS

The Swanson model, like a few of the material models, allows for the specification of thermal strain behavior within the material model itself, via the THERMAL EXPANSION FUNCTION command line. This command line, like the other “function-type” command lines in this model, requires that a function associated with the name be defined in the domain scope.

The bulk and shear scalings that can be used with the multilevel solver in Adagio are specified via a combination of the TARGET E, TARGET E FUNCTION, and MAX POISSONS RATIO command lines. If the TARGET E command line is not included (and the MAX POISSONS RATIO command line is included), the shear scaling is set to 1.0, and the bulk scaling is determined from the ratio of the scaled bulk modulus to its unscaled value, where the scaled bulk modulus is computed using the value of the max_poissons_ratio parameter along with the unscaled shear modulus. On the other hand, if both the TARGET E command line and the MAX POISSONS RATIO are included, bulk and shear scaling values are computed using scaled moduli that are calculated from the target_e and max_poissons_ratio parameter values.

Including the TARGET E FUNCTION command line allows time-dependent bulk and shear scaling to be used. If this command line is not specified, the bulk and shear scalings remain constant in solution time. If the command line is specified, the target Young’s modulus that is used for computing the scaled moduli is multiplied by the function value.

The REFERENCE STRAIN command line supplies a value for the reference strain used to create a normalized material constraint violation that is based on strains. Specifying a reference strain implies the use of strains for measuring the material constraint violation (or part of the control-stiffness error in Adagio). Otherwise, the material constraint violation is determined using the change in the scaled stress response over the current model problem.

Brief documentation on the theoretical basis for the Swanson model is given in Reference 12.
**4.2.22 Viscoelastic Swanson Model**

```
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value

#
BEGIN PARAMETERS FOR MODEL VISCOELASTIC_SWANSON
  YOUNGS MODULUS = <real>youngs_modulus
  POISSONS RATIO = <real>poissons_ratio
  BULK MODULUS = <real>bulk_modulus
  SHEAR MODULUS = <real>shear_modulus
  LAMBDA = <real>lambda
  A1 = <real>a1
  P1 = <real>p1
  B1 = <real>b1
  Q1 = <real>q1
  C1 = <real>c1
  R1 = <real>r1
  CUT OFF STRAIN = <real>ecut
  THERMAL EXPANSION FUNCTION = <string>eth_function_name
  PRONY SHEAR INFINITY = <real>ginf
  PRONY SHEAR 1 = <real>g1
  PRONY SHEAR 2 = <real>g2
  PRONY SHEAR 3 = <real>g3
  PRONY SHEAR 4 = <real>g4
  PRONY SHEAR 5 = <real>g5
  PRONY SHEAR 6 = <real>g6
  PRONY SHEAR 7 = <real>g7
  PRONY SHEAR 8 = <real>g8
  PRONY SHEAR 9 = <real>g9
  PRONY SHEAR 10 = <real>g10
  SHEAR RELAX TIME 1 = <real>tau1
  SHEAR RELAX TIME 2 = <real>tau2
  SHEAR RELAX TIME 3 = <real>tau3
  SHEAR RELAX TIME 4 = <real>tau4
  SHEAR RELAX TIME 5 = <real>tau5
  SHEAR RELAX TIME 6 = <real>tau6
  SHEAR RELAX TIME 7 = <real>tau7
  SHEAR RELAX TIME 8 = <real>tau8
  SHEAR RELAX TIME 9 = <real>tau9
  SHEAR RELAX TIME 10 = <real>tau10
  WLF COEF C1 = <real>wlf_c1
  WLF COEF C2 = <real>wlf_c2
  WLF TREF = <real>wlf_tref
  NUMERICAL SHIFT FUNCTION = <string>ns_function_name
  TARGET E = <real>target_e
  TARGET E FUNCTION = <string>etar_function_name
  MAX POISSONS RATIO = <real>max_poissons_ratio
```
4.2. MODEL SPECIFICATIONS

REFERENCE STRAIN = <real>reference_strain
END [PARAMETERS FOR MODEL VISCOELASTIC_SWANSON]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

The viscoelastic Swanson model is a finite strain viscoelastic model that has an initial elastic response that matches the Swanson material model. The bulk response is elastic, while the shear response is viscoelastic. This model is commonly employed in simulating the response of rubber materials. The viscoelastic Swanson model can be used in both Presto and Adagio. When the model is used in Adagio, it can be used with or without the control-stiffness option in Adagio’s multilevel solver for nearly incompressible materials where Poisson’s ratio, \( \nu \), \( \approx 0.5 \). The control-stiffness option is implemented via the CONTROL STIFFNESS command block and is discussed in Chapter 3 of the Adagio user’s guide. In the course of solving a series of model problems in Adagio, the material response from this model incorporates scaling the bulk and/or shear behaviors to yield a material response that is more amenable to solution using Adagio’s conjugate gradient solver. The final material behavior that is calculated corresponds to the actual moduli that are specified. When this model is used in Presto, the material scalings are ignored.

For a viscoelastic Swanson material, a viscoelastic Swanson command block starts with the input line:

```
BEGIN PARAMETERS FOR MODEL VISCOELASTIC_SWANSON
```

and terminates with an input line of the following form:

```
END [PARAMETERS FOR MODEL VISCOELASTIC_SWANSON]
```

In the above command blocks:

- The density of the material is defined with the DENSITY command line.
- Only two of the following elastic constants are required to define the unscaled bulk behavior:
  
  - Young’s modulus is defined with the YOUNGS MODULUS command line.
  - Poisson’s ratio is defined with the POISSONS RATIO command line.
  - The bulk modulus is defined with the BULK MODULUS command line.
  - The shear modulus is defined with the SHEAR MODULUS command line.
  - Lambda is defined with the LAMBDA command line.

- The following command lines are required:
  
  - The material constant A1 is defined with the A1 command line.
  - The material constant P1 is defined with the P1 command line.
  - The material constant B1 is defined with the B1 command line.
  - The material constant Q1 is defined with the Q1 command line.
  - The material constant C1 is defined with the C1 command line.
- The material constant R1 is defined with the \texttt{R1} command line.
- The small-strain value used for computing the glassy shear modulus is defined with the \texttt{CUT OFF STRAIN} command line.

- The \texttt{THERMAL EXPANSION FUNCTION} command line references the name of a function defined in a \texttt{DEFINITION FOR FUNCTION} command line in the domain scope that describes the linear thermal expansion as function of temperature. See the usage discussion below.

- \texttt{PRONY SHEAR INFINITY} command line. This command line is required.

- The normalized relaxation spectra coefficients are specified with the \texttt{PRONY SHEAR I} command lines, where the value of I varies sequentially from 1 to 10. These command lines are optional.

- The normalized relaxation spectra time constants are specified with the \texttt{SHEAR RELAX TIME I} command lines, where the value of I varies sequentially from 1 to 10. These command lines are optional.

- \texttt{WLF COEF C1} command line. This command line is required.

- \texttt{WLF COEF C2} command line. This command line is required.

- \texttt{WLF TREF} command line. This command line is required.

- \texttt{NUMERICAL SHIFT FUNCTION} command line. This command line is optional.

- The following material-scaling command lines are used only in Adagio:

  - The target Young’s modulus is defined with the \texttt{TARGET E} command line. This command line is required. See the usage discussion below.

  - The \texttt{TARGET E FUNCTION} command line references the name of a function defined in a \texttt{DEFINITION FOR FUNCTION} command line in the domain scope that describes the time variation of the target Young’s modulus. This command line is required. See the usage discussion below.

  - The maximum Poisson’s ratio is defined with the \texttt{MAX POISSONS RATIO} command line. This command line is required. See the usage discussion below.

  - The reference strain is defined with the \texttt{REFERENCE STRAIN} command line. This command line is required. See the usage discussion below.

As noted previously, only two of the elastic constants are required to define the unscaled bulk behavior. Together, the values for parameters in the \texttt{A1, P1, B1, Q1, C1, and R1} command lines define the unscaled glassy shear behavior, so these command lines must be present. The unscaled glassy shear modulus is determined from those parameter values along with the value of the parameter in the \texttt{CUT OFF STRAIN} command line, so this command line must also be present.

The viscoelastic Swanson model, like a few of the material models, allows for the specification of thermal strain behavior within the material model itself, via the \texttt{THERMAL EXPANSION}
FUNCTION command line. This command line, like the other “function-type” command lines in this model requires that a function associated with the name be defined in the domain scope.

The bulk and shear scalings that can be used with the multilevel solver in Adagio are specified via a combination of the TARGET E, TARGET E FUNCTION, and MAX POISSONS RATIO command lines. If the TARGET E command line is not included (and the MAX POISSONS RATIO command line is included), the shear scaling is set to 1.0, and the bulk scaling is determined from the ratio of the scaled bulk modulus to its unscaled value, where the scaled bulk modulus is computed using the value of the max_poissons_ratio parameter along with the unscaled shear modulus. On the other hand, if both the TARGET E command line and the MAX POISSONS RATIO command line are included, bulk and shear scaling values are computed using scaled moduli that are calculated from the target_e and max_poissons_ratio parameter values.

Including the TARGET E FUNCTION command line allows time-dependent bulk and shear scaling to be used. If this command line is not specified, the bulk and shear scalings remain constant in solution time. If the command line is specified, the target Young’s modulus that is used for computing the scaled moduli is multiplied by the function value.

The REFERENCE STRAIN command line supplies a value for the reference strain used to create a normalized material constraint violation that is based on strains. Specifying a reference strain implies the use of strains for measuring the material constraint violation (or part of the control-stiffness error in Adagio). Otherwise, the material constraint violation is determined using the change in the scaled stress response over the current model problem.

Brief documentation on the theoretical basis for the viscoelastic Swanson model is given in References 12, 13, 14, and 15.
4.3 Equation-of-State Model Specifications

This section describes material models that are applicable only for use in Presto.
4.3.1 Mie-Gruneisen Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  # {thermal strain option}
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL MIE_GRUNEISEN
    RHO_0 = <real>density
    C_0 = <real>sound_speed
    SHUG = <real>const_shock_velocity
    GAMMA_0 = <real>ambient_gruneisen_param
    POISSR = <real>poissons_ratio
    Y_0 = <real>yield_strength
    PMIN = <real>mean_stress(REAL_MAX)
  END [PARAMETERS FOR MODEL MIE_GRUNEISEN]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

The Mie-Gruneisen material model describes the nonlinear pressure-volume (or equivalently pressure-density) response of solids or fluids in terms of a reference pressure-volume curve and deviations from the reference curve in energy space. The reference curve is taken to be the experimentally determined principal Hugoniot, which is the locus of end states that can be reached by a shock transition from the ambient state. For details about this model, see Reference 16.

For Mie-Gruneisen energy-dependent materials, the Mie-Gruneisen command block begins with the input line:

BEGIN PARAMETERS FOR MODEL MIE_GRUNEISEN

and is terminated with an input line of the following form:

END [PARAMETERS FOR MODEL MIE_GRUNEISEN]

In the above command blocks:

- The {thermal strain option} is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.

- The ambient density, $\rho_0$, is defined with the RHO_0 command line. The ambient density is the density at which the mean pressure is zero, not necessarily the initial density.

- The ambient bulk sound speed, $c_0$, is defined by the C_0 command line. The ambient bulk sound speed is also the first constant in the shock-velocity-versus-particle-velocity relation...
\[ D = c_0 + Su, \] where \( u \) is the particle velocity. (See the following description of the \texttt{SHUG} command line for the definition of \( S \).)

- The second constant in the shock-velocity-versus-particle-velocity equation, \( S \), is defined by the \texttt{SHUG} command line. The shock-velocity-versus-particle-velocity relation is \( D = c_0 + Su \), where \( u \) is the particle velocity. (See the previous description of the \texttt{C\_0} command line for the definition of \( c_0 \).)

- The ambient Gruneisen parameter, \( \Gamma_0 \), is defined by the \texttt{GAMMA\_0} command line.

- Poisson’s ratio, \( \nu \), is defined by the \texttt{POISSR} command line. Poisson’s ratio is assumed constant.

- The yield strength, \( y_0 \), is defined by the \texttt{Y\_0} command line. The yield strength is zero for the hydrodynamic case.

- The fracture stress is defined by the \texttt{PMIN} command line. The fracture stress is a mean stress or pressure, so it must be negative or zero. This is an optional parameter; if not specified, the parameter defaults to \texttt{REAL\_MAX} (no fracture).

For information about the Mie-Gruneisen model, consult Reference 16.
4.3. Mie-Gruneisen Power-Series Model

```plaintext
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name

# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION = <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION = <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION = <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL MIE_GRUNEISEN_POWER_SERIES
RHO_0 = <real>density
C_0 = <real>sound_speed
K1 = <real>power_series_coeff1
K2 = <real>power_series_coeff2
K3 = <real>power_series_coeff3
K4 = <real>power_series_coeff4
K5 = <real>power_series_coeff5
GAMMA_0 = <real>ambient_gruneisen_param
POISSR = <real>poissons_ratio
Y_0 = <real>yield_strength
PMIN = <real>mean_stress(REAL_MAX)
END [PARAMETERS FOR MODEL MIE_GRUNEISEN_POWER_SERIES]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
```

The Mie-Gruneisen power-series model describes the nonlinear pressure-volume (or equivalently pressure-density) response of solids or fluids in terms of a reference pressure-volume curve and deviations from the reference curve in energy space. The reference curve is taken to be the experimentally determined principal Hugoniot, which is the locus of end states that can be reached by a shock transition from the ambient state. The Mie-Gruneisen power-series model is very similar to the Mie-Gruneisen model, except that the Mie-Gruneisen model bases the Hugoniot pressure-volume response on the assumption of a linear shock-velocity-versus-particle-velocity relation, while the Mie-Gruneisen power-series model uses a power-series expression. For details about this model, see Reference 16.

For Mie-Gruneisen power-series energy-dependent materials, the Mie-Gruneisen power-series command block begins with the input line:

```plaintext
BEGIN PARAMETERS FOR MODEL MIE_GRUNEISEN_POWER_SERIES
```

and is terminated an input line of the following form:

```plaintext
END [PARAMETERS FOR MODEL MIE_GRUNEISEN_POWER_SERIES]
```

In the above command blocks:

- The `{thermal strain option}` is used to define thermal strains. See Section 4.1.2.1 and
Section 4.1.2.2 for further information on defining and activating thermal strains.

- The ambient density, $\rho_0$, is defined with the \texttt{RHO}_0 \texttt{command line. The ambient density is the density at which the mean pressure is zero, not necessarily the initial density.}

- The ambient bulk sound speed, $c_0$, is defined by the \texttt{C}_0 \texttt{command line.}

- The power-series coefficients $k_1, k_2, k_3, k_4, \text{ and } k_5$ are defined by the command lines \texttt{K1}, \texttt{K2}, \texttt{K3}, \texttt{K4}, \text{ and } \texttt{K5}, respectively. Only the nonzero power-series coefficients need be input, since coefficients not specified will default to zero.

- The ambient gruneisen parameter, $\Gamma_0$, is defined by the \texttt{GAMMA}_0 \texttt{command line.}

- Poisson’s ratio, $\nu$, is defined by the \texttt{POISSR} \texttt{command line. Poisson’s ratio is assumed constant.}

- The yield strength, $y_0$, is defined by the \texttt{Y}_0 \texttt{command line. The yield strength is zero for the hydrodynamic case.}

- The fracture stress is defined by the \texttt{PMIN} \texttt{command line. The fracture stress is a mean stress or pressure, so it must be negative or zero. This is an optional parameter; if not specified, the parameter defaults to \texttt{REAL}_\texttt{MAX} \texttt{(no fracture).}

For information about the Mie-Gruneisen power-series model, consult Reference 16.
4.3.3 JWL (Jones-Wilkins-Lee) Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
 # {thermal strain option}
 THERMAL STRAIN FUNCTION = <string>thermal_strain_function
 # or all three of the following
 THERMAL STRAIN X FUNCTION =
 <string>thermal_strain_x_function
 THERMAL STRAIN Y FUNCTION =
 <string>thermal_strain_y_function
 THERMAL STRAIN Z FUNCTION =
 <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL JWL
 RHO_0 = <real>initial_density
 D = <real>detonation_velocity
 E_0 = <real>init_chem_energy
 A = <real>jwl_const_pressure1
 B = <real>jwl_const_pressure2
 R1 = <real>jwl_const_nondim1
 R2 = <real>jwl_const_nondim2
 OMEGA = <real>jwl_const_nondim3
 XDET = <real>x_detonation_point
 YDET = <real>y_detonation_point
 ZDET = <real>z_detonation_point
 TDET = <real>time_of_detonation
 B5 = <real>burn_width_const(2.5)
 END [PARAMETERS FOR MODEL JWL]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

The JWL model describes the pressure-volume-energy response of the gaseous detonation products of HE (High Explosive). For details about this model, see Reference 16.

For JWL energy-dependent materials, the JWL command block begins with the input line:

BEGIN PARAMETERS FOR MODEL JWL

and is terminated an input line of the following form:

END [PARAMETERS FOR MODEL JWL]

In the above command blocks:

- The {thermal strain option} is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.

- The initial density of the unburned explosive, \( \rho_0 \), is given by the RHO_0 command line.

- The detonation velocity, \( D \), is given by the D command line.
- The initial chemical energy per unit mass in the explosive, $E_0$, is given by the $E_0$ command line. Most compilations of JWL parameters give $E_0$ in units of energy per unit volume, rather than energy per unit mass. Thus, the tabulated value must be divided by $\rho_0$, the initial density of the unburned explosive.

- The JWL constants with units of pressure, $A$ and $B$, are given by the $A$ and $B$ command lines, respectively.

- The dimensionless JWL constants, $R_1$, $R_2$, and $\omega$, are given by the $R1$, $R2$, and $OMEGA$ command lines, respectively.

- The $x$-coordinate of the detonation point, $x_D$, is given by the $XDET$ command line.

- The $y$-coordinate of the detonation point, $y_D$, is given by the $YDET$ command line.

- The $z$-coordinate of the detonation point, $z_D$, is given by the $ZDET$ command line.

- The time of detonation, $t_D$, is given by the $TDET$ command line.

- The burn-width constant, $B_5$, is given by the $B5$ command line. The burn-width constant has a default value of 2.5.

For information about the JWL model, consult Reference 16.
4.3. EQUATION-OF-STATE MODEL SPECIFICATIONS

4.3.4 Ideal Gas Model

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
   # {thermal strain option}
   THERMAL STRAIN FUNCTION = <string>thermal_strain_function
   # or all three of the following
   THERMAL STRAIN X FUNCTION =
      <string>thermal_strain_x_function
   THERMAL STRAIN Y FUNCTION =
      <string>thermal_strain_y_function
   THERMAL STRAIN Z FUNCTION =
      <string>thermal_strain_z_function
   #
   BEGIN PARAMETERS FOR MODEL IDEAL_GAS
      RHO_0 = <real>initial_density
      C_0 = <real>initial_sound_speed
      GAMMA = <real>ratio_specific_heats
   END [PARAMETERS FOR MODEL IDEAL_GAS]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

The ideal gas model provides a material description based on the ideal gas law. For details about this model, see Reference 16.

For ideal gas materials, the ideal gas command block begins with the input line:

BEGIN PARAMETERS FOR MODEL IDEAL_GAS

and is terminated with an input line of the following form:

END [PARAMETERS FOR MODEL IDEAL_GAS]

In the above command blocks:

- The {thermal strain option} is used to define thermal strains. See Section 4.1.2.1 and Section 4.1.2.2 for further information on defining and activating thermal strains.

- The initial density, \( \rho_0 \), is given by the RHO_0 command line.

- The initial sound speed, \( c_0 \), is given by the C_0 command line.

- The ratio of specific heats, \( \gamma \), is given by the GAMMA command line.

For information about the ideal gas model, consult Reference 16.
4.4 Energy Deposition

BEGIN PRESCRIBED ENERGY DEPOSITION
  # {block set commands}
  BLOCK = <string_list>block_names
  INCLUDE ALL BLOCKS
  REMOVE BLOCK
  #
  # function commands
  T FUNCTION = <string>t_func_name
  X FUNCTION = <string>x_func_name
  Y FUNCTION = <string>y_func_name
  Z FUNCTION = <string>z_func_name
  #
  # input mesh command
  READ VARIABLE = <string>mesh_var_name
  #
  # user subroutine commands
  ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
  # {other user subroutine command lines}
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
END [PRESCRIBED ENERGY DEPOSITION]

The PRESCRIBED ENERGY DEPOSITION command block applies a set quantity of energy to energy-dependent material models for a given set of element blocks. Energy deposition represents a particular type of boundary condition, and thus this command block follows the general specification of command blocks used to specify boundary conditions in Chapter 6. The PRESCRIBED ENERGY DEPOSITION command block must appear in the region scope.

There are three options for defining the energy deposition for a set of elements: with standard SIERRA functions, with a mesh variable in the input mesh file, and by a user subroutine. If the energy deposition is a reasonably simple description and can be defined using the standard SIERRA functions, the function option is recommended. If the energy deposition requires a more complex description, it is necessary to use either the input mesh option or the user subroutine option. Only one of the three options can be specified in the command block.

The PRESCRIBED ENERGY DEPOSITION command block contains four groups of commands: block set, function, input mesh, and user subroutine. Each of these command groups, with the exception of the T FUNCTION command line, is basically independent of the others. Following are descriptions of the different command groups.
4.4. ENERGY DEPOSITION

4.4.1 Block Set Commands

The \{block set commands\} portion of the PRESCRIBED ENERGY DEPOSITION command block defines a set of element blocks associated with the prescribed energy deposition and can include some combination of the following command lines:

```
BLOCK = <string_list>block_names
INCLUDE ALL BLOCKS
REMOVE BLOCK
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of blocks. See Section 6.1.1 for more information about the use of these command lines for creating a set of blocks used in the command block. Either the BLOCK command line or the INCLUDE ALL BLOCKS command line must be present in the command block.

4.4.2 Function Commands

If the function option is used, all four function-type command lines, each referencing a user-defined function, must be included in the command block.

Following are the command lines related to the function option:

```
T FUNCTION = <string>t_func_name
X FUNCTION = <string>x_func_name
Y FUNCTION = <string>y_func_name
Z FUNCTION = <string>z_func_name
```

Each of the above command lines references a function name (defined in the domain scope in a DEFINITION FOR FUNCTION command block). All the functions referenced in these four command lines must appear in the domain scope.

The T FUNCTION command line gives the name of the user-defined $T$ function. The $T$ function describes how the applied input energy dose is integrated over time $t$. The $T$ function should be 0 at the start time and 1 at the time at which all energy is deposited. The $T$ function must be monotonically increasing over the time it is defined. The $T$ function describes the total percentage of energy that is deposited at a given time.

The X FUNCTION, Y FUNCTION, and Z FUNCTION command lines define three functions, which we will denote as $X$, $Y$, and $Z$, respectively. The $X$, $Y$, and $Z$ functions describe the total amount of energy to be deposited in an element as a function of position. Suppose we have element $A$ with centroid $(A_x, A_y, A_z)$. The total energy that will have been deposited in element $A$ at time $t$ is given by:

$$E_A = X(A_x)Y(A_y)Z(A_z)T(t),$$  \hspace{1cm} (4.7)

where $E_A$ is the total energy deposited.
4.4.3 Input Mesh Command

If the input mesh option is used, the quantity of energy deposited for each element will be read from an element variable defined in the mesh file.

Following is the command line related to the input mesh option:

```
READ VARIABLE = <string>mesh_var_name
```

The string `mesh_var_name` must match the name of an element variable in the mesh file that defines the energy deposition. Suppose that the total energy to be deposited for element \( A \) is \( v(A) \). The quantity of energy deposited at time \( t \) is then given by:

\[
E_A = v(A)T(t). \tag{4.8}
\]

The \( T \) function in Equation (4.8) is the same as that described in Section 4.4.2.

4.4.4 User Subroutine Commands

The user subroutine option allows for a very general description of the energy deposition, but this option requires that you write a user subroutine to implement this capability. The subroutine will be called by Presto at the appropriate time to generate the energy deposition.

Energy deposition uses an element subroutine signature. The subroutine returns one value per element for all the elements selected by use of the `{block set commands}`. The returned value is the current energy flux at an element at a given time. The output flags array is ignored. The total energy deposited in an element is found by a time integration of the returned subroutine fluxes. See Chapter 9 for more information about user subroutines.

Following are the command lines related to the user subroutine option:

```
ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

The user subroutine option is invoked by using the `ELEMENT BLOCK SUBROUTINE` command line. The string `subroutine_name` is the name of a FORTRAN subroutine written by the user. The other command lines listed here (`SUBROUTINE DEBUGGING OFF`, `SUBROUTINE DEBUGGING ON`, `SUBROUTINE REAL PARAMETER`, `SUBROUTINE INTEGER PARAMETER`, and `SUBROUTINE STRING PARAMETER`) are described in Section 9.2.2. Examples of using these command lines are provided throughout Chapter 9.
4.5 References


Chapter 5

Elements

This chapter explains how material, geometric, and other properties are associated with the various element blocks in a mesh file. A mesh file contains, for the most part, only topological information about elements. For example, there may be a group of elements in the mesh file that consists of four nodes defining a planar facet in three-dimensional space. Whether or not these elements are used as shells or membranes in our actual model of an object is determined by command lines in the input file. The specifics of a material type associated with these four node facets are also set in the input file.

Most elements can be used in either Presto or Adagio. If an element is available in one code but not the other, this information will be noted for the element. There is a special element implementation in Presto referred to as smoothed particle hydrodynamics (SPH). There is a section for SPH in the Presto manual but not in the Adagio manual. This chapter also includes descriptions of the commands for mass property calculations, element death, and mesh rebalancing. Two “element-like” capabilities are discussed in Chapter 5—torsional springs and rigid bodies. Although torsional springs and rigid bodies exhibit element-like behavior, they are really implemented as boundary conditions. From a user viewpoint, it is best to discuss the torsional-spring and rigid-body capabilities with elements.

Highlights of chapter contents follow. Section 5.1 discusses the FINITE ELEMENT MODEL command block, which provides the description of a mesh that will be associated with the elements. Section 5.2 presents the section command blocks that are used to define the different element sections. Next are descriptions of command blocks that exhibit element-like functionality. Section 5.3.1 explains the use of rigid bodies. Section 5.3.2 describes how to implement a torsional spring mechanism in Presto. In Section 5.4, the MASS PROPERTIES command block is described, which lets the user compute the total mass of the model or the mass of subparts of the model once the element blocks are completely defined in terms of geometry and material. Section 5.5 details the ELEMENT DEATH command block, which lets the user delete (kill) elements based on various criteria during an analysis. Three command blocks for derived quantities that are used, under certain conditions, with a command line in ELEMENT DEATH are discussed in Section 5.6. Finally, Section 5.7 presents various options for partitioning a mesh for parallel runs with Presto. The partitioning scheme can greatly influence the run time for a particular analysis. The command block for selecting a partitioning scheme is REBALANCE. The REBALANCE references a
ZOLTAN \textbf{PARAMETERS} command block. The \textbf{ZOLTAN \textbf{PARAMETERS}} command block sets various parameters that control the partitioning.

Most of the command blocks and command lines described next appear within the domain scope. There are some exceptions, and these exceptions are noted.

\section{Finite Element Model}

\begin{verbatim}
BEGIN FINITE ELEMENT MODEL <string>mesh_descriptor
  DATABASE NAME = <string>mesh_file_name
  DATABASE TYPE = <string>database_type(exodusII)
  ALIAS <string>mesh_identifier AS <string>user_name
  OMIT BLOCK <string>block_list
  COMPONENT SEPARATOR CHARACTER = <string>separator
  BEGIN PARAMETERS FOR BLOCK <string list>block_names
    #
    # Command lines that define attributes for
    # a particular element block appear in this
    # command block.
    #
    END [PARAMETERS FOR BLOCK <string list>block_names]
END [FINITE ELEMENT MODEL <string>mesh_descriptor]
\end{verbatim}

The input file must point to a mesh file that is to be used for an analysis. The name of the mesh file appears within a \textbf{FINITE ELEMENT MODEL} command block, which appears in the domain scope. In this command block, you will identify the particular mesh file that describes your model. Also within this command block, there will be one or more \textbf{PARAMETERS FOR BLOCK} command blocks. (All the \textbf{PARAMETERS FOR BLOCK} command blocks are embedded in the \textbf{FINITE ELEMENT MODEL} command block.) Within the \textbf{PARAMETERS FOR BLOCK} command block, you will set a material type and model, a section, and various other parameters for the element block. The concept of “section” is explained in Section 5.1.2.

The current element library is as follows:

- Eight-node, uniform-gradient hexahedron: Both a midpoint-increment formulation \cite{1} and a strongly objective formulation are implemented \cite{2}. These elements can be used with any of the material models described in Chapter 4, including the equation of state (EOS) models.

- Eight-node, selective-deviatoric hexahedron: Only a strongly objective formulation is provided. This element can be used with any of the material models described in Chapter 4 except the EOS models.

- Four-node tetrahedron: There is now the regular element formulation for the four-node tetrahedron and a node-based formulation for the four-node tetrahedron. For the regular element formulation, only a strongly objective formulation is implemented. The concept of a node-based four-node tetrahedron is described in Reference 3. The regular four-node tetrahedron
can be used with any of the material models described in Chapter 4 except the EOS models. The node-based tetrahedron can be used with any of the material models described in Chapter 4, including the EOS models.

- Eight-node tetrahedron: This tetrahedral element has nodes at the four vertices and nodes on the four faces. The eight-node tetrahedron has only a strongly objective formulation [4]. The eight-node tetrahedron uses a mean quadrature formulation even though it has the additional nodes. This element can be used with any of the material models described in Chapter 4, including the EOS models.

- Ten-node tetrahedron: Only a strongly objective formulation is implemented. This element can be used with any of the material models described in Chapter 4, including the EOS models.

- Four-node, quadrilateral, uniform-gradient membrane: Both a midpoint-increment formulation and a strongly objective formulation are implemented. This element is derived from the Key-Hoff shell formulation [5]. The strongly objective formulation has not been extensively tested, and it is recommended that the midpoint-increment formulation, which is the default, be used for this element type. These elements can be used with any of the following material models described in Chapter 4:
  - Elastic
  - Elastic-plastic
  - Elastic-plastic power-law hardening
  - Multilinear elastic-plastic hardening (no failure)

- Four-node, quadrilateral shell: This shell uses the Key-Hoff formulation [5]. Both a midpoint-increment formulation and a strongly objective formulation are implemented. The strongly objective formulation has not been extensively tested, and it is recommended that the midpoint-increment formulation, which is the default, be used for this element type. These elements can be used with any of the following material models described in Chapter 4:
  - Elastic
  - Elastic-plastic
  - Elastic-plastic power-law hardening
  - Multilinear elastic-plastic hardening without failure
  - Multilinear elastic-plastic hardening with failure

- Four-node, quadrilateral, selective-deviatoric membrane: Only a midpoint-increment formulation is implemented. These elements can be used with any of the following material models described in Chapter 4:
  - Elastic
  - Elastic-plastic
– Elastic-plastic power-law hardening
– Multilinear elastic-plastic hardening (no failure)

- (ONLY PRESTO) Two-node beam: The beam element is a uniform result model. Strains and stresses are computed only at the midpoint of the element. These midpoint values determine the forces and moments for the beam. There are five different sections currently implemented for the beam: rod, tube, bar, box, and I. This element can be used with any of the following material models described in Chapter 4:

  – Elastic
  – Elastic-plastic

- Two-node truss: The two-node truss element carries only a uniform axial stress. Currently, there is a linear-elastic material model for the truss element.

- Two-node spring: The two-node spring element computes a uniaxial resistance force based on a non-linear force-engineering strain function. This element can handle preloads, mass per unit length, resetting of the initial length after preload and any arbitrary loading function.

- Two-node damper: (Code Usage: Presto only) The two-node damping element computes a damping force based on the relative velocity of the two nodes along the axis of the element. This element uses only a damping parameter for a material property.

- Point mass: (Code Usage: Presto only) The point mass element allows the user to put a specified mass (and a mass only) at a node. This element requires input for density and an elastic material, but does not make use of the elastic material properties.

- Smoothed particle hydrodynamics (SPH) elements: These are one-dimensional elements. These elements can be used with any of the material models described in Chapter 4, including the EOS models.

The command block to describe a mesh file begins with

```
BEGIN FINITE ELEMENT MODEL <string>mesh_descriptor
```

and is terminated with:

```
END [FINITE ELEMENT MODEL <string>mesh_descriptor]
```

where `mesh_descriptor` is a user-selected name for the mesh. In this section, we will first discuss the command lines within the scope of the `FINITE ELEMENT MODEL` command block but outside the scope of the `PARAMETERS FOR BLOCK` command block. We will then discuss the `PARAMETERS FOR BLOCK` command block and the associated command lines for this particular block.
5.1. **FINITE ELEMENT MODEL**

5.1.1 **Identification of Mesh File**

Nested within the `FINITE ELEMENT MODEL` command block are two command lines (`DATABASE NAME` and `DATABASE TYPE`) that give the mesh name and define the type for the mesh file, respectively. The command line

```
DATABASE NAME = <string>mesh_file_name
```

gives the name of the mesh file with the string `mesh_file_name`. If the current mesh file is in the default directory and is named `job.g`, then this command line would appear as:

```
DATABASE NAME = job.g
```

If the mesh file is in some other directory, the command line would have to show the path to that directory. For parallel runs, the string `mesh_file_name` is the base name for the spread of parallel mesh files. For example, for a four-processor run, the actual mesh files associated with a base name of `job.g` would be `job.g.4.0`, `job.g.4.1`, `job.g.4.2`, and `job.g.4.3`. The database name on the command line would be `job.g`.

If the mesh file does not use the Exodus II format, you must specify the format for the mesh file using the command line:

```
DATABASE TYPE = <string>database_type(exodusII)
```

Currently, only the Exodus II database format is supported by Presto and Adagio for mesh input. Other options may be added in the future.

5.1.1.1 **Alias**

It is possible to associate a user-defined name with some mesh entity. The mesh entity names for Exodus II entities are typically the concatenation of the entity type (for example, “block”, “nodeset”, or “surface”), an underscore (“_”), and the entity id. This generated name can be aliased to a more descriptive name by using the `ALIAS` command line:

```
ALIAS <string>mesh_identifier AS <string>user_name
```

This alias can then be used in other locations in the input file in place of the Exodus II name. Examples of this association are as follows:

```
Alias block_1 as Case
Alias block_10 as Fin
Alias block_12 as Nose
Alias surface_1 as Nose_Case_Interface
Alias surface_2 as OuterBoundary
```

The above examples use the Exodus II naming convention described in Section 1.5.
5.1.1.2 Omit Block

If the finite element mesh contains element blocks that should be omitted from the finite element analysis, the OMIT BLOCK line command is used.

OMIT BLOCK <string>block_list

The element blocks listed in the command are removed from the model. Any nodesets or surfaces only existing on nodes or elements in the omitted element blocks are also omitted. Note that if this command is used in a parallel analysis, it is possible for the resulting model to become unbalanced if, for example, the omitted element blocks make up a large portion of the elements on one or more processors. In this case, the mesh can be rebalanced using the REBALANCE command described in Section 5.7.1.

Examples of omitting element blocks are:

Omit Block block_1 block_2
Omit Block block_10

5.1.1.3 Component Separator Character

A variable defined on the mesh database can be used as a prescribed energy deposition, an initial condition, or a prescribed temperature with the READ VARIABLE command. If the variable is a vector or a tensor, then the base name of the variable will be separated from the suffixes with a separator character. The default separator character is an underscore, but it can be changed with the COMPONENT SEPARATOR CHARACTER command.

COMPONENT SEPARATOR CHARACTER = <string>character|NONE

For example, the variable displacement can have the suffixes x, y, etc. By default, the base name is separated from the suffixes with an underscore character so that we have displacement_x, displacement_y, etc. in the mesh file. The underscore can be replaced as the default separator by using the above command line. If the data used the period as the separator, then the command would be

COMPONENT SEPARATOR CHARACTER = .

For the displacement example the components would then appear in the mesh file as displacement.x, displacement.y, etc.

The separator can be eliminated with an empty string or NONE.

5.1.2 Descriptors of Element Blocks

BEGIN PARAMETERS FOR BLOCK <string list>block_names
  MATERIAL <string>material_name
  SOLID MECHANICS USE MODEL <string>model_name
  SECTION = <string>section_id


5.1. FINITE ELEMENT MODEL

The finite element model consists of one or more element blocks. Associated with an element block or group of element blocks will be a PARAMETERS FOR BLOCK command block, which is also referred to in this document as an element-block command block. The basic information about the element blocks (number of elements, topology, connectivity, etc.) is contained in a mesh file. Specific attributes for an element block must be specified in the input file. If for example, a block of eight-node hexahedra is to use the selective-deviatoric versus mean-quadrature formulation, then the selective-deviatoric formulation must be specified in the input file. The element library is listed at the beginning of Section 5.1.

The element-block command block begins with the input line

```
BEGIN PARAMETERS FOR BLOCK <string list>block_names
```

and is terminated with the input line:

```
END [PARAMETERS FOR BLOCK <string list>block_names]
```

Here block_names is the list of element blocks assigned to the element-block command block. If the format for the mesh file is Exodus II, the typical form of a block_name is block_integerid, where integerid is the integer identifier for the block. If the element block is 280, the value of block_name would be block_280. It is also possible to generate an alias identifier for the element block and use this for the block_name. If block_280 is aliased to AL6061, then block_name becomes AL6061.

All the element blocks listed on the PARAMETERS FOR BLOCK command line will have the same mechanics properties. The mechanics properties are set by use of the various command lines. One of the key command lines, i.e., MATERIAL, will let you associate a material with the elements in the block. Another key command line is the SECTION command line. This command line lets you differentiate between elements with the same topology but different formulations. For example, assume that the topology of the elements in a block is a four-node quadrilateral. With the SECTION command line you can specify whether the element block will be used as a membrane or a shell. The SECTION command line also lets you assign a variety of parameters to an element, depending
on the element formulation.

It is important to state here that the SECTION command line only specifies an identifier that maps to a section command block that is defined by the user. There are currently several kinds of section command blocks for the different elements: SOLID SECTION, SHELL SECTION, MEMBRANE SECTION, BEAM SECTION, TRUSS SECTION, SPRING SECTION, DAMPER SECTION, POINT MASS SECTION, and SPH SECTION. It is within a section command block that the formulation-specific entities related to a particular element are specified. If no SECTION command line is present in an element-block command block, the code assumes the element block is a block of eight-node hexahedra using mean quadrature and the midpoint-increment formulation.

In addition to the material- and section-related command lines in an element-block command block, there are a number of other command lines. There are, for example, two command lines, HOURGLASS STIFFNESS, and HOURGLASS VISCOSITY, that will let you specify hourglass control parameters for the elements in the block (if these elements use hourglass control). These two command lines will overwrite the default hourglass control parameters for all elements in the block.

All the command lines that can be used for the element-block command block are described in Section 5.1.2.1 through Section 5.1.2.7. The various section command blocks are described in Section 5.2. The section command blocks and their related command lines are much easier to understand once the element-block command lines are described.

5.1.2.1 Material Property

MATERIAL <string>material_name
SOLID MECHANICS USE MODEL <string>model_name

The material property specification for an element block is done by using the above two command lines. The property specification references both a PROPERTY SPECIFICATION FOR MATERIAL command block and a material-model command block, which has the general form PARAMETERS FOR MODEL model_name. These command blocks are described in Chapter 4. The PROPERTY SPECIFICATION FOR MATERIAL command block contains all the parameters needed to define a material, and is associated with an element block (PARAMETERS FOR BLOCK command block) by use of the MATERIAL command line. Some of the material parameters inside the property specification are grouped on the basis of material models. A material-model command block is associated with an element block by use of the SOLID MECHANICS USE MODEL command line.

Consider the following example. Suppose there is a PROPERTY SPECIFICATION FOR MATERIAL command block with a material_name of steel. Embedded within this command block for steel is a material-model command block for an elastic model of steel and an elastic-plastic model of steel. Suppose that for the current element block we would like to use the material steel with the elastic model. Then the element-block command block would contain the input lines:

MATERIAL steel
SOLID MECHANICS USE MODEL elastic
If, on the other hand, we would like to use the material steel with the elastic-plastic model, the element-block command block would contain the input lines:

\begin{verbatim}
MATERIAL steel
SOLID MECHANICS USE MODEL elastic_plastic
\end{verbatim}

The user should remember that not all material types can be used with all element types.

### 5.1.2.2 Section

\[ \text{SECTION} = \text{<string>section_id} \]

The section specification for an element-block command block is done by using the above command line. The \text{section_id} is a string associated with a section command block. The various section command blocks are described in Section 5.2.

Suppose you wanted the current element-block command block to use the membrane formulation. You would define a \text{MEMBRANE SECTION} command block with some name, such as \text{membrane_rubber}. Inside the current element-block command block you would have the command line:

\begin{verbatim}
SECTION = membrane_rubber
\end{verbatim}

The thickness of the membrane would be described in the \text{MEMBRANE SECTION} command block and then associated with the current element-block command block.

There can be only one \text{SECTION} command line in an element-block command block. Each element-block command block within the model description can reference a unique section command block, or several element-block command blocks can reference the same section command block. For example, in Figure 5.1, the section named \text{membrane_rubber} appears in two different \text{PARAMETERS FOR MODEL} command blocks, but there is only one specification for their associated \text{MEMBRANE SECTION} command block. When several element-block command blocks reference the same section, the input file is less verbose, and it is easier to maintain the input file.

### 5.1.2.3 Linear and Quadratic Bulk Viscosity

\begin{verbatim}
LINEAR BULK VISCOSITY =
<real>linear_bulk_viscosity_value(0.06)
QUADRATIC BULK VISCOSITY =
<real>quad_bulk_viscosity_value(1.20)
\end{verbatim}

The linear and quadratic bulk viscosity are set with these two command lines. Consult the documentation for the elements [6] for a description of the bulk viscosity parameters.
5.1.2.4 Hourglass Control

HOURGLASS STIFFNESS = <real>hour_glass_stiff_value(solid = 0.05, shell/membrane = 0.0)
HOURGLASS VISCOSITY = <real>hour_glass_visc_value(solid = 0.0, shell/membrane = 0.0)

These two command lines set the hourglass control parameters for elements that use hourglass control. Currently, the included elements are the eight-node, uniform-gradient hexahedral elements; the eight-node and ten-node tetrahedral elements; and the four-node membrane and shell elements. Consult the element documentation [6] for a description of the hourglass parameters.

The hourglass stiffness parameter defaults to 0.05 for solids using hourglass control; it defaults to 0.0 for shell and membrane elements. A reasonable user defined hourglass stiffness (if needed) for shells and membranes is 0.005 (approximately an order of magnitude lower than for solid elements). The hourglass viscosity parameter defaults to 0.0 for all elements currently using hourglass control.

The hourglass stiffness is the same as the dilatational hourglass parameter, and the hourglass viscosity is the same as the deviatoric hourglass parameter.

The computation of the hourglass parameters can be strongly affected by the method that computes the effective moduli. The command line in Section 5.1.2.5 selects the method for computing the effective moduli.
5.1. **FINITE ELEMENT MODEL**

5.1.2.5 **Effective Moduli Model**

\[
\text{EFFECTIVE MODULI MODEL} = \text{<string>PRESTO|PRONTO|CURRENT|ELASTIC(PRONO)}
\]

The hourglass force computations require a measure of the material moduli to ensure appropriate scaling of the hourglass forces. For elastic, isotropic material models, the moduli are constant throughout the analysis. However, for nonlinear materials, the moduli are typically computed numerically from the stresses. For models with softening regimes or that approach perfect plasticity, the moduli may be difficult to define, and the way in which they are computed may adversely affect the analysis. Through the EFFECTIVE MODULI MODEL command line, Presto provides several methods for the computation of these effective moduli:

- **PRESTO**: This method includes a number of techniques for returning reasonable moduli for softening and perfectly plastic materials. The effective moduli that this approach produces are stiffer than those computed by the PRONTO approach.

- **PRONTO**: This method is the default and is identical to the method of computing effective moduli present in the Pronto3D code. It is similar to the PRESTO approach but generally produces moduli that are softer than the PRESTO approach.

- **CURRENT**: This method computes the effective moduli without any extra handling of negative or near-zero moduli cases. It generally provides the softest response but is also less stable.

- **ELASTIC**: This method simply uses the initial elastic moduli for the entire analysis. It is the most robust but also the most stiff, and may produce an overly stiff global response.

The EFFECTIVE MODULI MODEL command line should be used with caution because it can strongly affect the analysis results.

5.1.2.6 **Element Numerical Formulation**

\[
\text{ELEMENT NUMERICAL FORMULATION} = \text{<string>OLD|NEW(OLD)}
\]

For calculation of the critical time step, it is necessary to determine a characteristic length for each element. In one dimension, the correct characteristic element length is obviously the distance between the two nodes of the element. In higher dimensions, this length is usually taken to be the minimum distance between any of the nodes in the element. However, some finite element codes, primarily those based on Pronto3D [1], use as a characteristic length an eigenvalue estimate based on work by Flanagan and Belytschko [7]. That characteristic length provides a stable time step, but in many cases is far more conservative than the minimum distance between nodes. For a cubic element with side length equal to 1, and thus also surface area of each face and volume equal to 1, the minimum distance between nodes is 1. However, the eigenvalue estimate is \(1/\sqrt{3}\), which
is only 58% of the minimum distance. As the length of the element is increased in one direction while keeping surfaces in the lateral direction squares of area 1, the eigenvalue estimate asymptotes to $1/\sqrt{2}$ for very long elements. If the length is decreased, the eigenvalue estimate asymptotes to the minimum distance between nodes for very thin elements. In this case, the eigenvalue estimate is always more conservative than the minimum distance between nodes. However, consider an element whose cross section in one direction is not a square but a trapezoid with one side length much greater than the other. Assume the large side length is 1 and the other side length is arbitrarily small, $\varepsilon$. In this case, the minimum distance between nodes becomes $\varepsilon$, creating a very small and inefficient time step. However, the eigenvalue estimate is related to the length across the middle of the trapezoid, which for the conditions stated is $1/2$. Since both distances provide stable time steps, and one or the other can be much larger in various circumstances, the most efficient calculation is obtained by using the maximum of the two lengths, either the eigenvalue estimate or the minimum distance between nodes, to determine the time step.

By using the maximum of the lengths, the computed critical time step should be at the edge of instability, and the TIME STEP SCALE FACTOR command line should be used to provide a margin of safety. In this case the scale factor for the time step should not be greater than 0.9, and in some cases it may have to be reduced further. Thus, although the maximum of the lengths provides a time step that is closer to the critical value and provides better accuracy and efficiency, you may need to specify a smaller-than-expected scale factor for stability. For this reason, the choice of which approach to use is left to the user and is determined by the command line:

```
ELEMENT NUMERICAL FORMULATION = <string>OLD|NEW(OLD)
```

If the input parameter is OLD, only the eigenvalue estimate is used; NEW means that the maximum of the two lengths is used. The default is OLD so that users will have to specifically choose the new approach and be aware of the scale factor for the time step.

The ELEMENT NUMERICAL FORMULATION command line is applicable to both the energy-dependent and purely mechanical material models. If this command line is applied to blocks using energy-dependent materials, only the determination of the characteristic length is affected. If this command line is applied to an element block with a purely mechanical model and the OLD option is used, the Pronto3D-based artificial viscosity, time step, and eigenvalue estimate will be used in the element calculations. If, however, the NEW option is used, the artificial viscosity and time step will be computed from equations associated with the energy-dependent models. You should consult Reference 8 for further details about the critical time-step calculations and the use of this command line.

5.1.2.7 Activation/Deactivation of Element Blocks by Time

```
ACTIVE FOR PROCEDURE <string>proc_name DURING PERIODS
<string list>period_names
```

This command line permits the activation and deactivation of element blocks by time period. The time periods are defined in the TIME STEPPING BLOCK command block (Section 3.1.1) within a specific procedure named in a PRESTO PROCEDURE command block (Section 2.2.1). In the
ACTIVE FOR PROCEDURE command line, the element block is active for all periods listed for the named procedure. The element block is deactivated for all time periods that are absent from the list. If this command line is not used, then by default the block is active during all time periods. While this command line controls the activation and deactivation of all elements in a block, individual elements can be deactivated with the ELEMENT DEATH command block (see Section 5.5).
5.2 Element Sections

Element sections are defined by section command blocks. There are currently nine different types of section command blocks. The section command blocks appear in the domain scope, at the same level as the FINITE ELEMENT MODEL command block. In general, a section command block has the following form:

```
BEGIN section_type SECTION <string>section_name
  command lines dependent on section type
END [section_type SECTION <string>section_name]
```

Currently, `section_type` can be SOLID, SHELL, MEMBRANE, BEAM, TRUSS, SPRING, DAMPER, POINT MASS, or SPH. These various section types are identified as individual section command blocks and are described below. The corresponding `section_name` parameter in each of these command blocks, e.g., `truss_section_name` in the TRUSS SECTION command block, is selected by the user. The method used to associate these names with individual SECTION command lines in PARAMETERS FOR BLOCK command blocks is discussed in Section 5.1.2.2.

### 5.2.1 Solid Section

```
BEGIN SOLID SECTION <string>solid_section_name
  FORMULATION = <string>MEAN_QUADRATURE|
                 SELECTIVE_DEVIATORIC(MEAN_QUADRATURE)
  DEVIATORIC PARAMETER = <real>deviatoric_param
  STRAIN INCREMENTATION = <string>MIDPOINT_INCREMENT|
                          STRONGLY_OBJECTIVE|NODE_BASED(MIDPOINT_INCREMENT)
  NODE BASED ALPHA FACTOR = <real>bulk_stress_weight(0.01)
  NODE BASED BETA FACTOR = <real>shear_stress_weight(0.35)
  RIGID BODY = <string>rigid_body_name
  USE LAME
END [SOLID SECTION <string>solid_section_name]
```

The SOLID SECTION command block is used to specify the properties for solid elements (hexahedra and tetrahedra). This command block is to be referenced by an element block made up of solid elements. The two types of solid-element topologies currently supported are hexahedra and tetrahedra. The parameter `solid_section_name` is user-defined and is referenced by a SECTION command line in a PARAMETERS FOR BLOCK command block.

The FORMULATION command line specifies whether the element will use a single-point integration rule (mean quadrature) or a selective-deviatoric rule. The selective-deviatoric integration rule is a higher-order integration scheme, which is discussed below.

If the user wishes to use the selective-deviatoric rule, the DEVIATORIC PARAMETER command line must also appear in the SOLID SECTION command block. The selective-deviatoric parameter, `deviatoric_param`, which is valid from 0.0 to 1.0, indicates how much of the deviatoric
response should be taken from a uniform-gradient integration and how much should be taken from a full integration of the element. A value of 0.0 will give a pure uniform-gradient response with no hourglass control. Thus, this value is of little practical use. A value of 1.0 will give a fully integrated deviatoric response. Although any value between 0.0 and 1.0 is perfectly valid, lower values are generally preferred.

The selective-deviatoric elements, when used with a value greater than 0.0, provide hourglass control without artificial hourglass parameters.

Some of the solid elements support different strain-incrementation formulations. See the element summary at the beginning of Section 5.1 to determine what strain-incrementation formulations are available for the various elements. The `STRAIN_INCREMENTATION` command line, lets you specify a midpoint-increment strain formulation (`MIDPOINT_INCREMENT`), a strongly objective strain formulation (`STRONGLY_OBJECTIVE`), or a node-based formulation (`NODE_BASED`) for some of the elements. Consult the element documentation [2,6] for a description of these strain formulations.

The node-based formulation can only be used with four-node tetrahedral elements. If your element-block command block (i.e., a `PARAMETERS FOR BLOCK` command block) has a `SECTION` command line that references a `SOLID SECTION` command block that uses:

```
STRAIN_INCREMENTATION = NODE_BASED
```

then the element block must be a block of four-node tetrahedral elements.

The node-based formulation lets you calculate a solution that is some mixture of an element-based formulation (information from the center of an element) and a node-based formulation (information at a node that is based on all elements attached to the node). The node-based tetrahedron allows the user to model with four-node tetrahedral elements and avoid the main problems with regular tetrahedral elements. Regular tetrahedral elements are much too stiff and can produce very inaccurate results.

You can adjust the mixture of node-based versus element-based information incorporated into your solution with the `NODE_BASED ALPHA FACTOR` and `NODE_BASED BETA FACTOR` command lines. These two lines apply only if you have selected the `NODE_BASED` option on the `STRAIN_INCREMENTATION` command line. The value for `bulk_stress_weight` on the `NODE_BASED ALPHA FACTOR` command line sets the element bulk stress weighting factor, while the value for `shear_stress_weight` on the `NODE_BASED BETA FACTOR` command line sets the element shear stress weighting factor. You should consult Reference 3 to better understand the use of these weighting factors. If both of these factors are set to 0.0, you will be using a strictly node-based formulation. If both of these factors are set to 1.0, you will be using a strictly element-based formulation.

You can indicate that elements using this section should be rigid by including the `RIGID BODY` command line. The `RIGID BODY` command line specifies an identifier that maps to a rigid body command block. Consult with Section 5.3.1 for a full discussion of how to create rigid bodies.

You can request that the material model that will be used with this solid section come from the LAME material model library [9] with the `USE LAME` line command.
5.2.2 Shell Section

BEGIN SHELL SECTION <string>shell_section_name
THICKNESS = <real>shell_thickness
THICKNESS MESH VARIABLE =
  <string>THICKNESS|<string>var_name
THICKNESS TIME STEP = <real>time_value
THICKNESS SCALE FACTOR = <real>thick_scale_factor(1.0)
INTEGRATION RULE = TRAPEZOID|GAUSS|LOBATTO|SIMPSONS|
  USER(TRAPEZOID)
NUMBER OF INTEGRATION POINTS = <integer>num_int_points(5)
BEGIN USER INTEGRATION RULE
  <real>location_1 <real>weight_1
  <real>location_2 <real>weight_2
  ...
  <real>location_n <real>weight_n
END [USER INTEGRATION RULE]
LOFTING FACTOR = <real>lofting_factor(0.5)
ORIENTATION = <string>orientation_name
RIGID BODY = <string>rigid_body_name
END [SHELL SECTION <string>shell_section_name]

The SHELL SECTION command block is used to specify the properties for a shell element. If this command block is referenced in an element block of three-dimensional, four-node elements, the elements in the block will be treated as shell elements. The parameter, shell_section_name, is user-defined and is referenced by a SECTION command line in a PARAMETERS FOR BLOCK command block.

Either a THICKNESS command line or a THICKNESS MESH VARIABLE command line must appear in the SHELL SECTION command block.

If a shell element block references a SHELL SECTION command block with the command line:

  THICKNESS = <real>shell_thickness

then all the membrane elements in the block will have their thickness initialized to the value shell_thickness.

Presto can also initialize the thickness using an attribute defined on elements in the mesh file. Meshing programs such as PATRAN and CUBIT typically set the element thickness as an attribute on the elements. If the elements have one and only one attribute defined on the mesh, the THICKNESS MESH VARIABLE command line should be specified as:

  THICKNESS MESH VARIABLE = THICKNESS

which causes the thickness of the element to be initialized to the value of the attribute for that element. If there are zero attributes or more than one attribute, the thickness variable will not be automatically defined, and the command will fail.
The thickness may also be initialized by any other field present on the input mesh. To specify a field other than the single-element attribute, use this form of the THICKNESS MESH VARIABLE command line:

```
THICKNESS MESH VARIABLE = <string>var_name
```

Here, the string `var_name` is the name of the initializing field.

The input mesh may have values defined at more than one point in time. To choose the point in time in the mesh file that the variable should be read, use the command line:

```
THICKNESS TIME STEP = <real>time_value
```

The default time point in the mesh file at which the variable is read is 0.0.

Once the thickness of a shell element is initialized by using either the THICKNESS command line or the THICKNESS MESH VARIABLE command line, this initial thickness value can then be scaled using the scale-factor command line:

```
THICKNESS SCALE FACTOR = <real>thick_scale_factor
```

If the initial thickness of the shell is 0.15 inch, and the value for `thick_scale_factor` is 0.5, then the scaled thickness of the membrane will be 0.075.

The thickness mesh variable specification may be coupled with the THICKNESS SCALE FACTOR command line. In this case, the thickness mesh variable is scaled by the specified factor.

For shell elements, the user can select from a number of integration rules, including a user-defined integration option. The integration rule is selected with the command line:

```
INTEGRATION RULE = <string>TRAPEZOID|GAUSS|LOBATTO|SIMPSONS|
USER(TRAPEZOID)
```


The default integration scheme is TRAPEZOID with five integration points through the thickness. The number of integration points for TRAPEZOID can be set to any number greater than one by using the following command line:

```
NUMBER OF INTEGRATION POINTS = <integer>num_int_points(5)
```

The SIMPSONS, GAUSS, and LOBATTO integration schemes in the INTEGRATION RULE command line all default to five integration points. The number of integration points for these three schemes can be reset by using the NUMBER OF INTEGRATION POINTS command line. There are limitations on the number of integration points for some of these integration rules. The SIMPSONS rule can be set to any number greater than one, the GAUSS scheme can be set to one through seven integration points, and the LOBATTO integration scheme can be set to two through seven integration points.

In addition to these standard integration schemes, you may also define an integration scheme by using the USER INTEGRATION RULE command block.

```
BEGIN USER INTEGRATION RULE
  <real>location_1 <real>weight_1
```

END USER INTEGRATION RULE
You may NOT specify both a standard integration scheme and a user scheme. If the user option is specified in the integration rule command line, a set of integration locations with associated weight factors must be specified. This is done with tabular input command lines inside the user integration rule command block. The number of command lines inside this command block should match the number of integration points specified in the number of integration points command line. For example, suppose we wish to use a user-defined scheme with three integration points. The number of integration points command line should specify three (3) integration points and the number of command lines inside the user integration rule command block should be three (to give three locations and three weight factors).

For the user-defined rule, the integration point locations should fall between –1 and +1, and the weights should sum to 1.0.

The command line

\[
\text{LOFTING FACTOR} = \langle \text{real} \rangle \text{lofting\_factor}(0.5)
\]

allows the user to shift the location of the midsurface of a shell element relative to the geometric location of the shell element. By default, the geometric location of a shell element in a mesh represents the midsurface of the shell. If a shell has a thickness of 0.2 inch, the top surface of the shell is 0.1 inch above the geometric surface defined by the shell element, and the bottom surface of the shell is 0.1 inch below the geometric surface defined by the shell element. (The top surface of the shell is the surface with a positive element normal; the bottom surface of the shell is the surface with a negative element normal.)

Figure 5.2 shows an edge-on view of shell elements with a thickness of \( t \) and the location of the geometric plane in relation to the shell surfaces for three different values of the lofting factor—0.0, 0.5, and 1.0. If you want to have the geometric surface defined by the shell correspond to the top surface of the shell element, set the lofting factor to 1.0. If you want to have the geometric surface defined by the shell correspond to the bottom surface of the shell element, set the lofting factor to 0.0. The geometric surface is midway between the top and bottom surfaces for a lofting factor of 0.5. Note that the default for this factor is 0.5.

Suppose that the lofting factor is set to 1.0 and the thickness of the shell is 0.2 inch. Let us measure distances to the shell surfaces (top and bottom) by measuring along the positive element normal. The top surface of the shell will be located at a distance of 0.0 inch from the geometric shell surface, and the bottom surface of the shell will be located at a distance of –0.2 inch from the geometric shell surface.

Both the shell mechanics and contact use shell lofting. See Section 7.2 for a discussion of lofting surfaces for shells and contact.

The ORIENTATION command line lets you select a coordinate system for output of stresses. The ORIENTATION option makes use of an embedded coordinate system \( rst \) associated with each shell.
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Figure 5.2: Location of geometric plane of shell for various lofting factors.

The rst coordinate system for a shell element is shown in Figure 5.3. The r-axis extends from the center of the shell to the midpoint of the side of the shell defined by nodes 1 and 2. The t-axis is located at the center of the shell and is normal to the surface of the shell at the center point. The s-axis is the cross-product of the t-axis and the r-axis. The rst-axes form a local coordinate system at the center of the shell; this local coordinate system moves with the shell element as the element deforms.

Figure 5.3: Local rst coordinate system for a shell element.

The ORIENTATION command line in the SHELL SECTION command block references an ORIENTATION command block that appears in the domain scope. As described in Chapter 2 of this document, the ORIENTATION command block can be used to define a local coordinate system $X''Y''Z''$ at the center of a shell element. In the original shell configuration (time 0), one of the axes—$X''$, $Y''$, or $Z''$—is projected onto the plane of the shell element. The angle between this projected axis of the
$X''Y''Z''$ coordinate system and the $r$-axis is used to establish the transformation for the stresses. We will illustrate this with an example.

Suppose that in our ORIENTATION command block we have specified a rotation of 30 degrees about the $1$-axis ($X'$-axis). The command line for this rotation in the ORIENTATION command block would be:

\[
\text{ROTATION ABOUT } 1 = 30
\]

For this case, we project the $Y''$-axis onto the plane of the shell (Figure 5.4). The angle between this projection and the $r$-axis establishes a transformation for the in-plane stresses of the shell (the stresses in the center of the shell lying in the plane of the shell). What will be output as the in-plane stress $\sigma_{xx}^{ip}$ will be in the $Y''$-direction; what will be output as the in-plane stress $\sigma_{yy}^{ip}$ will be in the $Z''$-direction. The in-plane stress $\sigma_{xy}^{ip}$ is a shear stress in the $Y''Z''$-plane. The $X''Y''Z''$ coordinate system maintains the same relative position in regard to the $rst$ coordinate system. This means that the $X''Y''Z''$ coordinate system is a local coordinate system that moves with the shell element as the element deforms.

![Figure 5.4: Rotation of 30 degrees about the 1-axis ($X'$-axis).](image)

The following permutations for output of the in-plane stresses occur depending on the axis (1, 2, or 3) specified in the ROTATION ABOUT command line:

- Rotation about the 1-axis ($X'$-axis): The in-plane stress $\sigma_{xx}^{ip}$ will be in the $Y''$-direction; the in-plane stress $\sigma_{yy}^{ip}$ will be in the $Z''$-direction. The in-plane stress $\sigma_{xy}^{ip}$ is a shear stress in the $Y''Z''$-plane.

- Rotation about the 2-axis ($Y'$-axis): The in-plane stress $\sigma_{xx}^{ip}$ will be in the $Z''$-direction; the in-plane stress $\sigma_{yy}^{ip}$ will be in the $X''$-direction. The in-plane stress $\sigma_{xy}^{ip}$ is a shear stress in the $Z''X''$-plane.
• Rotation about the 3-axis (Z’-axis): The in-plane stress $\sigma_{xx}^p$ will be in the $X''$-direction; the in-plane stress $\sigma_{yy}^p$ will be in the $Y''$-direction. The in-plane stress $\sigma_{xy}^p$ is a shear stress in the $X''Y''$-plane.

You can indicate that elements using this section should be rigid by including the RIGID BODY command line. The RIGID BODY command line specifies an indenter that maps to a rigid body command block. Consult with Section 5.3.1 for a full discussion of how to create rigid bodies.

5.2.3 Membrane Section

BEGIN MEMBRANE SECTION <string>membrane_section_name
  THICKNESS = <real>mem_thickness
  THICKNESS MESH VARIABLE =
  <string>THICKNESS|<string>var_name
  THICKNESS TIME STEP = <real>time_value
  THICKNESS SCALE FACTOR = <real>thick_scale_factor(1.0)
  FORMULATION = <string>MEAN_QUADRATURE|
  SELECTIVE_DEVIATORIC(MEAN_QUADRATURE)
  DEVIATORIC PARAMETER = <real>deviatoric_param
  LOFTING FACTOR = <real>lofting_factor(0.5)
  RIGID BODY = <string>rigid_body_name
END [MEMBRANE SECTION <string>membrane_section_name]

The MEMBRANE SECTION command block is used to specify the properties for a membrane element. If a section defined by this command block is referenced in the parameters for a block of four-noded elements, the elements in that block will be treated as membranes. The parameter membrane_section_name is user-defined and is referenced by a SECTION command line in a PARAMETERS FOR BLOCK command block.

Either a THICKNESS command line or a THICKNESS MESH VARIABLE command line must appear in the MEMBRANE SECTION command block.

If a membrane element block references a MEMBRANE SECTION command block with the command line:

  THICKNESS = <real>mem_thickness

then all the membrane elements in the block will have their thickness initialized to the value mem_thickness.

Presto can also initialize the thickness using an attribute defined on elements in the mesh file. Meshing programs such as PATRAN and CUBIT typically set the element thickness as an attribute on the elements. If the elements have one and only one attribute defined on the mesh, the THICKNESS MESH VARIABLE command line should be specified as:

  THICKNESS MESH VARIABLE = THICKNESS

which causes the thickness of the element to be initialized to the value of the attribute for that element. If there are zero attributes or more than one attribute, the thickness variable will not be
automatically defined, and the command will fail.

The thickness may also be initialized by any other field present on the input mesh. To specify a field other than the single-element attribute, use this form of the THICKNESS MESH VARIABLE command line:

\[
\text{THICKNESS MESH VARIABLE} = \langle \text{string}\rangle \text{var\_name}
\]

where the string \text{var\_name} is the name of the initializing field.

The input mesh may have values defined at more than one point in time. To choose the point in time in the mesh file that the variable should be read, use the command line:

\[
\text{THICKNESS TIME STEP} = \langle \text{real}\rangle \text{time\_value}
\]

The default time point in the mesh file at which the variable is read is 0.0.

Once the thickness of a membrane element is initialized by using either the THICKNESS command line or the THICKNESS MESH VARIABLE command line, this initial thickness value can then be scaled by using the scale-factor command line:

\[
\text{THICKNESS SCALE FACTOR} = \langle \text{real}\rangle \text{thick\_{-}scale\_factor}
\]

If the initial thickness of the membrane is 0.15 inch, and the value for \text{thick\_scale\_factor} is 0.5, then the scaled thickness of the membrane will be 0.075.

The FORMULATION command line specifies whether the element will use a single-point integration rule (mean quadrature) or a selective-deviatoric integration rule:

\[
\text{FORMULATION} = \langle \text{string}\rangle \text{MEAN\_QUADRATURE|SELECTIVE\_DEVIATORIC}
\]

(MEAN\_QUADRATURE)

The selective-deviatoric rule is a higher-order integration scheme, which is discussed below.

If the user wishes to use the selective-deviatoric rule, the DEVIATORIC PARAMETER command line must also appear in the MEMBRANE SECTION command block:

\[
\text{DEVIATORIC PARAMETER} = \langle \text{real}\rangle \text{deviatoric\_param}
\]

The selective-deviatoric parameter, \text{deviatoric\_param}, which is valid from 0.0 to 1.0, indicates how much of the deviatoric response should be taken from a uniform-gradient integration and how much should be taken from a full integration of the element. A value of 0.0 will give a pure uniform-gradient response with no hourglass control. Thus, this value is of little practical use. A value of 1.0 will give a fully integrated deviatoric response. Although any value between 0.0 and 1.0 is perfectly valid, lower values are generally preferred.

The selective-deviatoric elements, when used with a parameter greater than 0.0, provide hourglass control without artificial hourglass parameters.

The command line

\[
\text{LOFTING FACTOR} = \langle \text{real}\rangle \text{lofting\_factor}(0.5)
\]

allows the user to shift the location of the midsurface of a membrane element relative to the geometric location of the membrane element. By default, the geometric location of a membrane
element in a mesh represents the midsurface of the membrane. If a membrane has a thickness of 0.2 inch, the top surface of the membrane is 0.1 inch above the geometric surface defined by the membrane element, and the bottom surface of the membrane is 0.1 inch below the geometric surface defined by the membrane element. (The top surface of the membrane is the surface with a positive element normal; the bottom surface of the membrane is the surface with a negative element normal.)

Figure 5.2, which shows lofting for shells, is also applicable to membranes. For membranes, Figure 5.2 represents an edge-on view of membrane elements with a thickness of \( t \) and the location of the geometric plane in relation to the membrane surfaces for three different values of the lofting factor—0.0, 0.5, and 1.0. If you want to have the geometric surface defined by the membrane correspond to the top surface of the membrane element, set the lofting factor to 1.0. If you want to have the geometric surface defined by the membrane correspond to the bottom surface of the membrane element, set the lofting factor to 0.0. The geometric surface is midway between the top and bottom surfaces for a lofting factor of 0.5. Note that the default for this factor is 0.5.

Suppose that the lofting factor is set to 1.0 and the thickness of the membrane is 0.2 inch. Let us measure distances to the membrane surfaces (top and bottom) by measuring along the positive element normal. The top surface of the membrane will be located at a distance of 0.0 inch from the geometric membrane surface, and the bottom surface of the membrane will be located at a distance of –0.2 inch from the geometric membrane surface.

Both the membrane mechanics and contact use membrane lofting. See Section 7.2 for a discussion of lofting surfaces for membranes and contact.

You can indicate that elements using this section should be rigid by including the RIGID BODY command line. The RIGID BODY command line specifies an indenter that maps to a rigid body command block. Consult with Section 5.3.1 for a full discussion of how to create rigid bodies.
5.2.4 Beam Section

BEGIN BEAM SECTION <string>beam_section_name
   SECTION = <string>ROD|TUBE|BAR|BOX|I
   WIDTH = <real>section_width
   HEIGHT = <real>section_width
   WALL THICKNESS = <real>wall_thickness
   FLANGE THICKNESS = <real>flange_thickness
   T AXIS = <real>tx <real>ty <real>tz (0 0 1)
   REFERENCE AXIS = <string>CENTER|RIGHT|TOP|LEFT|BOTTOM(CENTER)
   AXIS OFFSET = <real>s_offset <real>t_offset
   RIGID BODY = <string>rigid_body_name
END [BEAM SECTION <string>beam_section_name]

The BEAM SECTION command block is used to specify the properties for a beam element. If this command block is referenced in an element block of three-dimensional, two-node elements, the elements in the block will be treated as beam elements. The parameter, beam_section_name, is user-defined and is referenced by a SECTION command line in a PARAMETERS FOR BLOCK command block.

Five different cross sections can be specified for the beam—ROD, TUBE, BAR, BOX, and I—via use of the SECTION command line. Each section requires a specific set of command lines for a complete geometric description. The command lines related to section geometry are WIDTH, HEIGHT, WALL THICKNESS, and FLANGE THICKNESS. We present a summary of the geometric parameter command lines required for each section as a quick reference.

- If the section is ROD, the following geometry command lines are required:
  
  WIDTH = <real>section_width
  HEIGHT = <real>section_width

- If the section is TUBE, the following geometry command lines are required:

  WIDTH = <real>section_width
  HEIGHT = <real>section_width
  WALL THICKNESS = <real>wall_thickness

- If the section is BAR, the following geometry command lines are required:

  WIDTH = <real>section_width
  HEIGHT = <real>section_width

- If the section is BOX, the following geometry command lines are required:

  WIDTH = <real>section_width
  HEIGHT = <real>section_width
  WALL THICKNESS = <real>wall_thickness
5.2. **ELEMENT SECTIONS**

- If the section is I, the following geometry command lines are required:

  ```
  WIDTH = <real>section_width
  HEIGHT = <real>section_width
  WALL THICKNESS = <real>wall_thickness
  FLANGE THICKNESS = <real>flange_thickness
  ```

All the sections require the **T AXIS** command line. The **REFERENCE AXIS** and **AXIS OFFSET** command lines are optional.

Before presenting details about the various sections, we will discuss the local coordinate system for the beam. (The geometric properties are related to this local coordinate system.) For the beam, it is necessary to specify a local Cartesian coordinate system, which will be designated as \( r \), \( s \), and \( t \). The \( r \)-axis lies along the length of the beam and passes through the centroid of the beam. The \( t \)-axis is specified by the user. The initial direction of the \( t \)-axis is specified by a vector in the global coordinate system. If we want the initial position of the \( t \)-axis to be parallel to the global Z-axis, then we would use the command line:

  ```
  T AXIS = 0 0 1
  ```

If we wanted the initial position of the \( t \)-axis to be parallel to a vector \((0.5, 0.8660, 0)\) in the global coordinate system, then we would use the command line:

  ```
  T AXIS = 0.5 0.8660 0.0
  ```

The \( t \)-axis will change position as the beam deforms (rotates about the \( r \)-axis). This change in position is tracked internally by the computations for the beam element. The \( s \)-axis is computed from the cross-product of the \( t \)-axis and the \( r \)-axis. The **HEIGHT** for the beam cross section is in the direction of the \( t \)-axis, and the **WIDTH** of the beam cross section is in the direction of the \( s \)-axis.

Now that the local coordinate system for the beam has been defined, we can describe the definition of each section.

- The **ROD** section is a solid elliptical section. The diameter along the height is specified by the **HEIGHT** command line, and the diameter along the width is specified by the **WIDTH** command line.

- The **TUBE** section is a hollow elliptical section. The diameter along the height is specified by the **HEIGHT** command line, and the diameter along the width is specified by the **WIDTH** command line. The wall thickness for the tube is specified by the **WALL THICKNESS** command line.

- The **BAR** section is a solid rectangular section. The height is specified by the **HEIGHT** command line, and the width is specified by the **WIDTH** command line.

- The **BOX** section is a hollow rectangular section. The height is specified by the **HEIGHT** command line, and the width is specified by the **WIDTH** command line. The wall thickness for the box is specified by the **WALL THICKNESS** command line.
• The I section is the standard I-section associated with a beam. The height of the I-section is given by the \texttt{HEIGHT} command line, and the width of the flanges is given by the \texttt{WIDTH} command line. The thickness of the vertical member is given by the \texttt{WALL THICKNESS} command line, and the thickness of the flanges is given by the \texttt{FLANGE THICKNESS} command line.

By default, the \( r \)-axis coincides with the geometric centerline of the beam. The geometric centerline of the beam is defined by the location of the two nodes defining the beam connectivity. It is possible to offset the local \( r \)-axis, \( s \)-axis, and \( t \)-axis from the geometric centerline of the beam. To do this, one can use either the \texttt{REFERENCE AXIS} command line or the \texttt{AXIS OFFSET} command line, but not both.

The \texttt{REFERENCE AXIS} command line has the options \texttt{CENTER}, \texttt{TOP}, \texttt{RIGHT}, \texttt{BOTTOM}, and \texttt{LEFT}. The \texttt{CENTER} option is the default, which means that the \( r \)-axis coincides with the geometric centerline of the beam. If the \texttt{TOP} option is used, the \( r \)-axis is moved in the direction of the original \( t \)-axis by a positive distance \( \text{HEIGHT}/2 \) from the centroid so that it passes through the top of the beam section (top being defined in the direction of the positive \( t \)-axis). If the \texttt{RIGHT} option is used, the \( r \)-axis is moved in the direction of the original \( s \)-axis by a positive distance \( \text{WIDTH}/2 \) so that it passes through the right side of the beam section (the section being viewed in the direction of the negative \( r \)-axis). If the \texttt{BOTTOM} option is used, the \( r \)-axis is moved in the direction of the original \( t \)-axis by a distance \( \text{HEIGHT}/2 \) so that it passes through the bottom of the beam section (bottom being defined in the direction of the negative \( t \)-axis). If the \texttt{LEFT} option is used, the \( r \)-axis is moved in the direction of the original \( s \)-axis by a negative distance \( \text{WIDTH}/2 \) so that it passes through the left side of the beam section (the section being viewed in the direction of the negative \( r \)-axis). For all options, the \( s \)-axis and the \( t \)-axis remain parallel to their original positions before the translation of the \( r \)-axis.

The \texttt{AXIS OFFSET} command line allows the user to offset the local coordinate system from the geometric centerline by an arbitrary distance. The first parameter on the command line moves the \( r \)-axis a distance \texttt{s_offset} from the centroid of the section along the original \( s \)-axis. The second parameter on the command line moves the \( r \)-axis a distance \texttt{t_offset} from the centroid of the section along the original \( t \)-axis. The \( s \)-axis and \( t \)-axis remain parallel to their original positions before the translation of the \( r \)-axis.

Strains and stresses are computed at the midpoint of the beam. The integration of the stresses over the cross section at the midpoint is used to compute the internal forces in the beam. Each beam section has its own integration scheme. The integration scheme for each of the sections is shown in Figure 5.5 through Figure 5.7. The numbers in these figures show the relative location of the integration points in regard to the centroid of the section and the \( s \)-axis and the \( t \)-axis.

At each integration point, there is an axial strain (with a corresponding axial stress) and an in-plane (in the plane of the cross section) shear strain (with a corresponding shear stress). The user can output this stress and strain information by using the \texttt{RESULTS OUTPUT} commands described in Chapter 8. The registered variable that will let users access the strain at the beam integration points is \texttt{beam_strain_inc}, and the registered variable that will let users access the stress at the beam integration points is \texttt{beam_stress}. If the user requests output for the beam strain, 32 values are given for the strain. The first value (designated in the output as 01) is the axial strain at the first
integration point, the second value (designated in the output as 02) is the shear strain at the first integration point, etc. The odd values for the strain output (01, 03, 05, etc.) are the axial strains at the integration points. The even values of the strain output (02, 04, 06, etc.) are the shear strains at the integration points. For the case where there are only nine integration points (the rod), only the first 18 values for strain have any meaning for the section (the values 19 through 32 are zero). For the I-section, only the first 30 of the strain values have meaning since this section only has 15 integration points. For all other sections, all 32 values have meaning. A pattern similar to that for the strains holds for stresses.

As an alternative for the stress output, you may use the registered variables `beam_stress_axial` and `beam_stress_shear`. The variable `beam_stress_axial` contains only the axial stresses. The first value associated with `beam_stress_axial` (designated as 01) corresponds to the axial stress at integration point 1, the second value associated with `beam_stress_axial` (designated as 02) corresponds to the axial stress at integration point 2, and so on. The variable `beam_stress_shear` contains only shear stresses. The correlation between numbering the values for `beam_stress_shear` (01, 02, ...) and the integration points is the same as for `beam_stress_axial`.

It is possible to access mean values for the internal forces at the midpoint of the beam. The axial force at the midpoint of the beam is obtained by referencing the registered variable `beam_axial_force`. The transverse forces at the midpoint of the beam in the s-direction and the t-direction are obtained by referencing `beam_transverse_force_s` and `beam_transverse_force_t`, respectively. The torsion at the midpoint of the beam (the moment about the r-axis), is obtained by referencing `beam_moment_r`. The moments about the s-axis and the t-axis are obtained by referencing `beam_moment_s` and `beam_moment_t`, respectively.

You can indicate that elements using this section should be rigid by including the RIGID BODY command line. The RIGID BODY command line specifies an indenter that maps to a rigid body command block. Consult with Section 5.3.1 for a full discussion of how to create rigid bodies.
5.2.5 Truss Section

BEGIN TRUSS SECTION <string>truss_section_name
    AREA = <real>cross_sectional_area
    INITIAL LOAD = <real>initial_load
    PERIOD = <real>period
    RIGID BODY = <string>rigid_body_name
END [TRUSS SECTION <string>truss_section_name]

The TRUSS SECTION command block is used to specify the properties for a truss element. If this command block is referenced in an element block of three-dimensional, two-node elements, the elements in the block will be treated as truss elements. The parameter, truss_section_name, is user-defined and is referenced by a SECTION command line in a PARAMETERS FOR BLOCK command block.

The cross-sectional area for truss elements is specified by the AREA command line. The value cross_sectional_area is the cross-sectional area of the truss members in the element block.

The truss can be given some initial load over some given time period. The magnitude of the load is specified by the INITIAL LOAD command line. If the load is compressive, the sign on the value initial_load should be negative; if the load is tensile, the sign on the value initial_load should be positive. The period is specified by the PERIOD command line.

The initial load is applied over some period by specifying the axial strain rate in the truss, $\varepsilon$, over some period $p$. At some given time $t$, the strain rate is

$$\dot{\varepsilon} = \frac{ap}{2} \left[ 1 - \cos \left( \frac{\pi t}{p} \right) \right], \quad (5.1)$$

where
In Equation (5.2), $F_i$ is the initial load, $E$ is the modulus of elasticity for the truss, and $A$ is the area of the truss. Over the period $p$, the total strain increment generates the desired initial load in the truss.

During the initial load period, the time increments should be reasonably small so that the integration of $\dot{e}$ over the period is accurate. The period should be set long enough so that if the model was held in a steady state after time $p$, there would only be a small amount of oscillation in the load in the truss.

When doing an analysis, you may not want to activate certain boundary conditions until after the prestressing is done. During the prestressing, time-independent boundary conditions such as fixed displacement will most likely be turned on. Time-dependent boundary conditions such as prescribed acceleration or prescribed force will most likely be activated after the prestressing is complete.

You can indicate that elements using this section should be rigid by including the \texttt{RIGID BODY} command line. The \texttt{RIGID BODY} command line specifies an indenter that maps to a rigid body command block. Consult with Section 5.3.1 for a full discussion of how to create rigid bodies.

### 5.2.6 Spring Section

BEGIN SPRING SECTION <string>spring_section_name
FORCE STRAIN FUNCTION = <string>force_strain_function
DEFAULT STIFFNESS <real>default_stiffness
PRELOAD = <real>preload_value
PRELOAD DURATION = <real>preload_duration
RESET INITIAL LENGTH AFTER PRELOAD = <string>NO|YES
MASS PER UNIT LENGTH = <real>mass_per_unit_length
END [SPRING SECTION <string>spring_section_name]

The **SPRING SECTION** command block is used to specify the properties for a spring element. If this command block is referenced in an element block of three-dimensional, two node elements, the elements in the block will be treated as spring elements. The parameter, *spring_section_name*, is user-defined and is referenced by a **SECTION** command line in a **PARAMETERS FOR BLOCK** command block.

The spring behavior is governed by the force-engineering strain function which is specified by the **FORCE STRAIN FUNCTION** command line. The force generated by the spring element is based on the evaluation of the user specified *force_strain_function*, which has units of $F$ vs $dL/L_0$ with the current engineering strain of the spring, $dL/L_0$. This allows the force-strain function to be length independent.

The **DEFAULT STIFFNESS** command block specifies the spring stiffness used during the first time step and during preload. In all other situations the spring stiffness is based on the slope of the force-strain function evaluated at the previous timestep and the current timestep. The unit of *default_stiffness* is force.

To specify a preload on the spring both the **PRELOAD** and **PRELOAD DURATION** command line must be specified. The **PRELOAD** command line specifies the magnitude of the preload force, while the **PRELOAD DURATION** command line specifies how long the preload application should take, in seconds.

An optional preload input, **RESET INITIAL LENGTH AFTER PRELOAD**, is used when the user would like the initial length of the spring to reset to the displaced length after the preload has occurred. If this command line is not specified, or is set to **NO**, the initial length of the spring is the undeformed length as calculated from the input mesh.

Springs can optionally have mass through the **MASS PER UNIT LENGTH** command line. However, this input parameter is required if the spring elements are not individual two-node elements, but rather a string of spring elements, where the inter-spring nodes are only connected to the two adjacent springs. It should be noted, if the mass per unit length is not specified there is no critical timestep calculated for the spring elements.

### 5.2.7 Damper Section

BEGIN DAMPER SECTION <string>damper_section_name
  AREA = <real>damper_cross_sectional_area
END [DAMPER SECTION <string>damper_section_name]

The **DAMPER SECTION** command block is used to specify the properties for a damper element. If this command block is referenced in an element block of three-dimensional, two-node elements, the elements in the block will be treated as damper elements. The parameter, *damper_section_
name, is user-defined and is referenced by a SECTION command line in a PARAMETERS FOR BLOCK command block.

The cross-sectional area for damper elements is specified by the DAMPER AREA command line. The value damper_cross_sectional_area is the cross-sectional area of the dampers in the element block.

The damper area is used only to generate mass associated with the damper element. The mass is the density for the damper element multiplied by the original volume of the element (original length multiplied by the damper area).

The force generated by the damper element depends on the relative velocity along the current direction vector for the damper element. If \( \mathbf{n} \) is a unit normal pointing in the direction from node 1 to node 2, if \( \mathbf{v}_1 \) and \( \mathbf{v}_2 \) are the velocity vectors at nodes 1 and 2, respectively, then the force generated by the damper element is

\[
F_d = \eta \mathbf{n} \cdot (\mathbf{v}_2 - \mathbf{v}_1),
\]

where \( \eta \) is the damping parameter. Currently, the damping parameter must be specified by using an elastic material model for the damper element. The value for Young’s modulus in the elastic material model is used for the damping parameter \( \eta \).

### 5.2.8 Point Mass Section

BEGIN POINT MASS SECTION <string>pointmass_section_name
  VOLUME = <real>volume
  RIGID BODY = <string>rigid_body_name
END [POINT MASS SECTION <string>pointmass_section_name]

A point mass element is simply a mass at a node, which can be a convenient modeling tool in certain instances. The user can create an element block with one or more point masses. Each point mass must be associated with an existing node. A point mass will have its mass added to the mass at the node. (Other mass at the node will be derived from mass due to elements attached to the node.) The mass at a node due to a point mass is treated like any other mass at a node derived from an element. The mass due to point mass will be included in body force calculations and kinetic energy calculations, for example.

Point masses are a convenient modeling tool to be used in conjunction with rigid bodies. An element block including one or more point masses can be included like any other element block in a collection of element blocks used to define a rigid body. The element block of point masses can be used to adjust the total mass and inertia properties for the rigid body. (The point mass element does not have to be used only in conjunction with rigid bodies. One can place a point mass at a node associated with solid or structural elements.)

If you have an element block in which the connectivity for each element is only one node, then you may use this element block as a collection of point masses. This command block would have the following form:
BEGIN PARAMETERS FOR BLOCK <string>block_id
  MATERIAL = <string>material_name
  SOLID MECHANICS USE MODEL <string>material_model_name
  SECTION = <string>point_mass_section_name
END PARAMETERS FOR BLOCK <string>block_id

The element block associated with our point mass must reference a material command block just like any other element block. The product of the density specified in the material block and the volume specified in the section block (for the point mass) will be taken as the mass of each point mass in the element block. Suppose, for example, you have the following PARAMETERS FOR BLOCK command block for an element block with point masses:

BEGIN PARAMETERS FOR BLOCK block_105
  MATERIAL = mass_for_pointmass
  SOLID MECHANICS USE MODEL elastic
  SECTION = pmass_1
END PARAMETERS FOR BLOCK block_105

The above element block for the point mass elements references the material mass_for_pointmass. Let the density associated with this material be 0.0153. Let the value of the volume parameter associated with the section block pmass_1 be 4.0. Each point mass in the element block will have a mass of $4.0 \times 0.0153 = 0.0612$.

If you have access to the SEACAS codes from Sandia National Laboratories, you may use the codes in this library to generate element blocks with point mass elements. See Reference 11 for an overview of the SEACAS codes. By using various SEACAS codes, you can easily generate an element block with one or more point masses. For each point mass in the element block, you should create an eight-node hexahedral element that is centered at the point where you want the point mass located. The hexahedron can have arbitrary dimensions, but it is best to work with a unit cube. Suppose you wanted a point mass at (13.5, 27.0, 3.1415). You could create a unit hexahedron (1 by 1 by 1) centered on (13.5, 27.0, 3.1415). The SEACAS program SPHGEN3D will convert the hexahedron to a zero-dimensional element in three-dimensional space located at the center of the hexahedron. For our specific example, the program SPHGEN3D would create a zero-dimensional element, basically an element consisting of a single node, at (13.5, 27.0, 3.1415).

You can indicate that elements using this section should be rigid by including the RIGID BODY command line. The RIGID BODY command line specifies an indenter that maps to a rigid body command block. Consult with Section 5.3.1 for a full discussion of how to create rigid bodies.

5.2.9 SPH Section

BEGIN SPH SECTION <string>sph_section_name
  RADIUS MESH VARIABLE = <string>var_name|<string>attribute|
  SPHERE INITIAL RADIUS = <real>rad
  RADIUS MESH VARIABLE TIME STEP = <string>time
SPH (smoothed particle hydrodynamics) is useful for modeling fluids or for modeling materials that undergo extremely large distortions. One must be careful when using SPH for modeling. SPH tends to exhibit both accuracy and stability problems, particularly in tension. An SPH particle interacts with other nearest-neighbor SPH particles based on radius properties of all the elements involved; SPH particles react with other elements, such as tetrahedra, hexahedra, and shells, through contact. You should consult Reference 10 regarding the theoretical background for SPH.

You can define contact interaction between the particles in an SPH element block and other element types. In order to do this, you must use the CONTACT NODE SET option described in Section 7.2.4. All of the particles in the SPH element block must be included in a node set if you use the CONTACT NODE SET option.

All the particles contained in an SPH element block must be given some initial radius. There are two options for setting the initial radius for each particle. First, each particle can be given the same radius. To set the radius for each particle in an element block to the same value, use the SPHERE INITIAL RADIUS command line. The parameter \( \text{rad} \) on this command line sets the radius for all the SPH particles in the element block. Second, the radius for each particle can be read from a mesh file. The radii can be read from a variable on the mesh file as the attributes associated with the element block. If you want to read some variable from the mesh file for the radii, then you would use:

\[
\text{RADIUS MESH VARIABLE} = \text{sph\_radius}
\]

where \( \text{sph\_radius} \) is the variable name on the mesh file. If you want to use the variable associated with a specific time on the mesh file, you should use the RADIUS MESH VARIABLE TIME STEP command line to select the specific time. If you want to read the attributes associated with the particles, then you should insert the command line

\[
\text{RADIUS MESH VARIABLE} = \text{attribute}
\]

(as shown) into the SPH SECTION command block. Pronto3d [1] only offers the attribute option. To compare Presto and Pronto3d results, you should use the attribute option.

Once SPH determines the initial radius (through either the SPHERE INITIAL RADIUS command line or the RADIUS MESH VARIABLE command line), it will recalculate the optimal radius for the particle. The initial radii must be such that each sphere will overlap at least a few other SPH elements. If the initial radii are too small, the optimal radius calculation will fail, and the particles will not interact. If the initial radii are too large, many interactions may need to be checked, and the initialization calculation for the optimal radius step may take a long time.

After the radii are initialized, you may determine whether the radii are to remain constant or are to change throughout the analysis. The CONSTANT SPHERE RADIUS command line is an optional command line that prevents the sphere radius from changing over the course of the calculation. By default, the sphere radii will expand or contract based on the changing density in the elements to satisfy the relation that element mass (a constant) equals element volume times element density. If the CONSTANT SPHERE RADIUS command line appears, then the radii for all particles will remain...
constant.

Your analysis problem using SPH may be inherently one-, two-, or three-dimensional. You may indicate whether or not there is some inherent dimensionality in the problem by using the `PROBLEM DIMENSION` command line. The possible value for this command line is 1 (one-dimensional), 2 (two-dimensional), or 3 (three-dimensional). The default value is 3 for three-dimensional. The internal SPH calculations are modified depending on the value set on the `PROBLEM DIMENSION` command line. If, for example, your problem is inherently two-dimensional in nature, you may get more accurate results by specifying the dimension for your problem as 2 (as opposed to 1 or 3).

**Utility Commands.** In addition to the SPH-related command lines just described (which appear in the `SPH SECTION` command block) there are two other SPH-related command lines:

```plaintext
SPH SYMMETRY PLANE <string>+X|+Y|+Z|-X|-Y|-Z
<real>position_on_axis(0.0)
SPH DECOUPLE STRAINS: <string>material1 <string>material2
```

If either one or both of these command lines are used, they should be placed directly into the domain scope. (All other SPH-related command lines must be nested within the `SPH SECTION` command block; the `SPH SECTION` command block, like all other section command blocks, is in the domain scope.) The symmetry conditions are applied to all SPH element blocks.

The `SPH SYMMETRY PLANE` command line may be used to reduce model sizes by specifying symmetry planes and modeling only a portion of the model. Due to the nonlocal nature of SPH element integration, symmetry planes cannot be defined with boundary conditions alone; these planes must be explicitly defined. A plane is defined by an outward normal vector aligned with one of the axes (+X, +Y, +Z, -X, -Y, -Z) and some point on the axis, which represents a point in the plane. Suppose for example, the outward normal to the plane of symmetry is in the negative Y-direction (-Y) and the plane of symmetry passes through the y-axis at y = +2.56. Then the definition for the symmetry plane would be:

```plaintext
SPH SYMMETRY PLANE -Y +2.56
```

The `SPH DECOUPLE STRAINS` command line prevents two dissimilar materials from directly interacting. Generally, the material properties at a particle are the average of the material properties from nearby particles. If particles with very dissimilar material properties are interacting, this interaction can create problems. The `SPH DECOUPLE STRAINS` command line ensures that particles with very dissimilar material properties do not directly interact by material-property averaging, but instead just interact with a contact-like interaction. The two material types that are not to interact are specified by the parameters `material1` and `material2`. These parameters will appear as material names on a `PROPERTY SPECIFICATION FOR MATERIAL` command block.

**Display.** For purposes of visualizing the element stresses, it may be necessary to copy these element variables into nodal variables. This can easily be done by defining a `USER VARIABLE` command block (Section 9.2.4) in conjunction with a `USER OUTPUT` command block (Section 8.1.2). Once the nodal variable is defined, it can be output in a `RESULTS OUTPUT` command block (Section 8.1.1). An example is provided below. The SPH element blocks for the problem are element blocks 20, 21, and 22. All other element blocks are non-SPH elements.
- In the domain scope:

```
BEGIN USER VARIABLE nodal_stress
    TYPE = NODE SYM_TENSOR LENGTH = 1
END
```

- In the region scope:

```
BEGIN USER OUTPUT
    BLOCK = block_20 block_21 block_22
    COPY ELEMENT VARIABLE rotated_stress TO NODAL VARIABLE nodal_stress
END

BEGIN RESULTS OUTPUT output_presto
    DATABASE NAME = sph.e
    DATABASE TYPE = exodusII
    AT TIME 0.0 INCREMENT = 1.0e-04
    NODAL VARIABLES = nodal_stress
END RESULTS OUTPUT output_presto
```
5.3 Element-like Functionality

This section describes functionality in Presto that resembles the previously described elements to some extent. This functionality is not really implemented using the element structure in Presto, however. The functionality described in this section—rigid bodies and the torsional spring mechanism—is specified through command blocks that appear in the domain scope Presto region, respectively.

5.3.1 Rigid Body

BEGIN RIGID BODY <string>rb_name
  MASS = <real>mass
  MASS LOCATION = <real>CGx <real>CGy <real>CGz
  INERTIA = <real>Ixx <real>Iyy <real>Izz <real>Ixy <real>Iyz <real>Izx
  POINT INERTIA = <real>Ixx <real>Iyy <real>Izz <real>Ixy <real>Iyz <real>Izx
  MAGNITUDE = <real>magnitude_of_velocity
  DIRECTION = <string>direction_definition
  ANGULAR VELOCITY = <real>omega
  CYLINDRICAL AXIS = <string>axis_definition
END [RIGID BODY <string>rb_name]

A rigid body can consist of any combination of elements—solid elements, structural elements, and point masses—except SPH elements. All nodes associated with a rigid body maintain their same relative position to each other as determined at time 0 when there is no deformation of the body. This means that the elements associated with the rigid body do not deform over time. These elements are free to move (rotate and translate) through space, but they cannot deform. Element blocks that are part of a rigid body can adjoin deformable element blocks. For any rigid body consisting of several element blocks, the element blocks defining the rigid body do not have to be contiguous. You may have more than one rigid body in a model.

Presto creates a new node for each rigid body in the analysis. The new nodes are true nodes in that they are associated with solution fields such as displacement, velocity, and rotational velocity. These nodes will appear in a results file along with other nodes. The global node number given to the new nodes is simply the total number of nodes in the mesh plus one, repeated for each new rigid body node.

If you construct a model where all the element blocks compose a rigid body, you will need to set an initial time in the TIME CONTROL command block (Section 3.1.1). Include the line:

INITIAL TIME STEP = 1.0e-6

If an element block is declared to be a part of a rigid body, the internal force calculations are not called for the elements in that block. Part of the internal force calculation for an element is an element time-step estimate. If all elements are in a rigid body, the element time-step computations are not performed, and there is no estimate for a global time step. You must supply an initial time step only if all the elements are part of a rigid body. If some elements are in a rigid body, but
others are not, then you will automatically obtain a valid time step estimate for the problem. If you must set an initial time step for your problem because all elements are in a rigid body, then you should not override the default value of 1.0 for the time step scale factor (see Section 3.1.1). The time step you set for this particular case (all elements in a rigid body) must remain constant. The value of $1.0 \times 10^{-6}$ should work well for most problems. Do not use an initial time step larger than $1.0 \times 10^{-6}$ as this could cause loss of accuracy in the solution of the problem.

To construct the rigid body, you will need to use the above command block, which appears in the domain scope, plus the `RIGID BODY` command line that appears in the various `SECTION` command blocks described in this chapter. Suppose, for example, `rigidbody_1` consists of element blocks 100, 110, and 280. The `PARAMETERS FOR BLOCK` command blocks for element blocks 100, 110, and 280 must all contain a `SECTION` command line. In each case, the Section referred to must contain a line such as:

```
RIGID BODY = rigidbody_1
```

Once you have declared an element block or some collection of element blocks to be a rigid body and created a rigid body name (through the Section chosen), that rigid body name must appear as the name in a `RIGID BODY` command block. In our example, we must have a `RIGID BODY` command block with the value for `rb_name` set to `rigidbody_1`. Therefore, at a minimum, you must have a command block in the domain with the form

```
BEGIN RIGID BODY rigidbody_1
END RIGID BODY rigidbody_1
```

for our example.

The `RIGID BODY` command block has several different command lines, composing essentially three groups of commands. One group consists of the `MASS`, `MASS LOCATION`, `POINT INERTIA`, and `INERTIA` command lines, a second group consists of the paired `MAGNITUDE` and `DIRECTION` command lines, and a third group consists of the paired `ANGULAR VELOCITY` and `CYLINDRICAL AXIS` command lines. Each of the three groups is optional. You can combine any of these groups in the command block, or you could have a command block that contains none of the command lines, whereupon you would only supply the value for `rb_name` in the block.

Input to the `MASS` command line consists of a single real number that defines the total mass of the rigid body. If this line command is not present, the mass of the rigid body will be computed using the elements in the rigid body and their densities.

The `MASS LOCATION` command line requires three real numbers. Using this line command will specify the center of mass for the rigid body. If this line command is not present, the center of mass will be calculated.

Input to the `INERTIA` command line also consists of six real numbers. If present, this command line will set the inertia for the rigid body. If it is not present, moments and products of inertia are computed for the rigid body based on the location of the center of mass of the rigid body and the element masses for all the elements associated with the rigid body.

Input to the `POINT INERTIA` command line consists of six real numbers that define moments ($I_{xx}, I_{yy}, I_{zz}$) and products ($I_{xy}, I_{yx}, I_{zx}$) of inertia to be added to the inertia tensor of the rigid body. This modified inertia tensor (rather than the inertia tensor based solely on element
mass) is then used to calculate the motion of the rigid body.

If the rigid body has an initial velocity in some direction, this should be specified with the **MAGNITUDE** and **DIRECTION** command lines. The **MAGNITUDE** command line gives the magnitude of the initial velocity applied to the center of mass of the rigid body, and the **DIRECTION** command line gives a defined direction for the initial velocity for the center of mass. All blocks associated with the rigid body should be given the same initial velocity by using an **INITIAL VELOCITY** command block. (The information in the RIGID BODY command block is only applied to the center of mass of the rigid body.)

If the rigid body has an initial rotation about some axis, this should be specified with the **ANGULAR VELOCITY** and **CYLINDRICAL AXIS** command lines. The **ANGULAR VELOCITY** command line gives the initial velocity of the center of mass of the rigid body due to an angular velocity about some defined axis given on the **CYLINDRICAL AXIS** command line. All blocks associated with the rigid body should be given the same initial angular velocity by using an **INITIAL VELOCITY** command block. (The information in the RIGID BODY command block is only applied to the center of mass of the rigid body.)

Presto automatically outputs quantities such as displacement for the center of mass of the rigid body. The name assigned to a rigid body will be used to construct registered variable names that give the quantities. This lets you identify the output associated with a rigid body based on the name you assigned for the rigid body.

Immediately before the results file is written, the accelerations for nodes associated with a rigid body are updated to reflect the accelerations due to the rigid-body constraints. This ensures that the accelerations sent to the results output are correct for a given time.

In summary, if you use a rigid body in an analysis, you will do one or more of the following steps:

- Create a rigid body using one or more element blocks (except SPH element blocks). A **RIGID BODY** command line must appear in the **SECTION** command block used in the **PARAMETERS FOR BLOCK** command block for any element block associated with a rigid body.

- Include point mass element blocks with the rigid body if appropriate. To include point mass element blocks in a rigid body, a **RIGID BODY** command line must appear in the **SECTION** command block used in the **PARAMETERS FOR BLOCK** command block for those point mass element blocks.

- Include a **RIGID BODY** command block in the domain.

- Associate an initial velocity or initial rotation about an axis with the rigid body, if appropriate. If any of the blocks associated with a rigid body have been given an initial velocity or initial rotation, the rigid body must have the same specification for the initial velocity or initial rotation.

- Output center-of-mass information for the rigid body.

The above steps involve a number of different command blocks. To demonstrate how to fully implement a rigid body, we will provide a specific example that exercises the various options available to a user.
Let us assume that we want to create a rigid body named `part_a` consisting of three element blocks. Two of the element blocks, element block 100 and element block 535, are eight-node hexahedra; one of the element blocks, element block 600, consists of only point masses. The RIGID BODY command block, SECTION command block, and the element blocks we want to associate with the rigid body will be as follows:

```plaintext
begin solid section hex_section
  rigid body = part_a
end
begin point mass section pm_section
  rigid body = part_a
  volume = 0.1
end
begin parameters for block block_100
  material = steel
  solid mechanics model use elastic
  section = hex_section
end
begin parameters for block block_535
  material = aluminum
  solid mechanics model use elastic
  section = hex_section
end
begin parameters for block block_600
  material = mass_for_pointmass
  solid mechanics model use elastic
  section = pm_section
end
```

To adjust the moments and products of inertia computed by Presto for the rigid body `part_a`, we included the POINT INERTIA command line in the above section command block for the rigid body.

Now that we have defined the rigid body, we will examine how to specify an initial angular velocity about an axis for the rigid body and how to output information at the center of mass for the rigid body. The center of mass of the rigid body is some computed point associated with the body. It may or may not be at or near any node in the body.

Suppose we want to have the rigid body spin at 600 radians/sec about an axis parallel to the x-axis and passing through a point at (0, 10, 20). We would define this axis using the following set of DEFINE command lines:

```plaintext
define direction parallel_to_x with vector 2.0 0.0 0.0
define point off_axis with coordinates 0.0 10.0 20.0
define axis body_axis with point off_axis
direction parallel to x
```
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The blocks in the rigid body will be given an initial angular velocity of 600 radians/sec about the above axis if we use the following command block for initial angular velocity:

```
begin initial velocity
  block = block_100 block_535 block_600
cylindrical axis = body_axis
  angular velocity = 600
end initial velocity
```

The RIGID BODY command block must be given the same specification for an initial angular velocity. The angular velocity specification in the RIGID BODY command block is applied to the center of mass of the rigid body to make sure its initial motion is consistent with the initial motion of all the nodes in the rigid body as defined by the INITIAL VELOCITY command block. Our RIGID BODY command block (in the region) will appear as follows:

```
begin rigid body part_a
  cylindrical axis = body_axis
  angular velocity = 600
end rigid body part_a
```

Presto automatically generates and outputs global data associated with the rigid body (e.g. displacement and quaternion). The displacement of the rigid body named part_a will be written to the results file with the name DISPLX_PART_A.

If you have more than one rigid body in your model, you will be able to keep track of the center-of-mass information based on the rigid body name you give to each rigid body.

5.3.2 Torsional Spring Mechanism

```
BEGIN TORSIONAL SPRING MECHANISM <string>spring_name
  NODE SETS = <string>nodelist_int1 <string>nodelist_int2
    <string>nodelist_int3 <string>nodelist_int4
  TORSIONAL STIFFNESS = <real>stiffness
  INITIAL TORQUE = <real>init_load
  PERIOD = <real>time_period
  ACTIVE PERIODS = <string list>period_names
END [TORSIONAL SPRING MECHANISM <string>spring_name]
```

This feature was originally implemented to model a torsional spring wrapped around a fixed pin. One end of the pin is fixed to a base, and one end of the spring is attached to this base. There is an arm on the other end of the pin, and this arm can rotate around the pin. The second end of the spring is attached to this arm. The spring resists motion of the arm. Any similar mechanism can be modeled with the torsional spring. Although the torsional spring is element-like in its overall behavior, its implementation within the code structure is different from the other elements described in Chapter 5. The torsional spring does not make use of a section, and its command
The mechanism consists of two nodes that represent the axis of a torsional spring. Node 0 is at the base of the torsional spring, and node 1 is at the top of the torsional spring. A third node, reference node 0, defines an arm extending from the axis of the torsional spring to some attachment point near the base of the spring. A fourth node, reference node 1, defines an arm extending from the axis of the torsional spring to some attachment point near the top of the spring. The rotation of the two arms relative to each other as measured along the axis of the torsional spring represents the angular deformation of the spring and determines the moment in the spring. The moment in the spring is translated into external forces at the two attachment points, reference node 0 and reference node 1.

In the TORSIONAL SPRING MECHANISM command block, the string spring_name is defined by the user. Via the NODE SETS command line, the mechanism is defined with four node sets, and each node set has a single node. The first set (nodelist_int1) defines node 0 in Figure 5.8; node 0 is the origin of a local coordinate system for the torsional spring mechanism. The second node set (nodelist_int2) defines node 1 in Figure 5.8; node 0 and node 1 define the axis of the torsional spring mechanism. The third node set (nodelist_int3) defines reference node 0; reference node 0 is an attachment point for the spring associated with node 0. The fourth node set (node_int4) defines reference node 1; reference node 1 is an attachment point for the spring associated with node 1.

The nodes defining the spring mechanism are used to set up a local coordinate system \((x', y', z')\). The \((z')\)-axis runs along the axis of the spring from node 0 to node 1. The \(x'\)-axis extends from the axis of the spring and passes through reference node 0. If we are looking down the axis of the spring in the negative \(z'\)-direction, a positive rotation of the arm defined by node 1 and reference node 1 is in the counterclockwise direction. This is shown in Figure 5.9.

The torque, \(T\), in the spring is simply
Figure 5.9: Positive direction of rotation for torsional spring.

\[ T = K\theta, \quad (5.4) \]

where \( K \) is the torsional stiffness and \( \theta \) is the rotation of the top arm relative to the bottom arm as measured along the axis of the spring. In the TORSIONAL STIFFNESS command line, \( K \) is specified by the real value stiffness.

The torque in the spring is converted to external forces with components in the global coordinate system XYZ. These external forces depend on the torque and the length of the spring arms. The length of the spring arms is automatically calculated.

You can apply an initial torque with the real value init_load in the INITIAL TORQUE command line. The maximum value of the torque is reached in the time specified by the real value time_period in the PERIOD command line.

The initial torque is applied over some period by specifying the angular rate of deformation in the torsional spring, \( \dot{\theta} \), over some period \( p \). At some given time \( t \), the angular rate of deformation is

\[ \dot{\theta} = \frac{a}{2} \frac{p}{\left[ 1 - \cos \left( \frac{\pi t}{p} \right) \right]}, \quad (5.5) \]

where

\[ a = \frac{2T_i}{Kp}. \quad (5.6) \]

In Equation (5.6), \( T_i \) is the initial torque. Over the period \( p \), the total strain increment generates the desired initial load in the truss.
During the initial load period, the time increments should be reasonably small so that the integration of $\dot{\theta}$ over the period is accurate. The period should be set long enough so that if the model was held in a steady state after time $p$, there would be only a small amount of oscillation in the load in the torsional spring.

When doing an analysis, you may not want to activate certain boundary conditions until after the prestressing is done. During the prestressing, time-independent boundary conditions such as fixed displacement will most likely be turned on. Time-dependent boundary conditions such as prescribed acceleration or prescribed force will most likely be activated after the prestressing is complete.

You can output the torque in the spring, the total rotation, and the last angle between the arms. The name specified on the command block is used to construct parameters for the mechanism. Suppose the input line is:

```
begin torsional spring mechanism lower_spring
```

where `lower_spring` is a user-specified name. The code will automatically generate the parameters `TS_lower_spring_MOMENT`, `TS_lower_spring_ROTATION`, and `TS_lower_spring_LAST_ANGLE`. These variables can then be output in a results file. For example, one could use

```
global variables = TS_lower_spring_MOMENT as ts_lspring_m
global variables = TS_lower_spring_ROTATION as ts_lspring_r
global variables = TS_lower_spring_LAST_ANGLE as ts_lspring_la
```

in the `RESULTS OUTPUT` command block. If several torsional spring mechanisms appear in one model, you can generate unique names to keep track of the parameters associated with each spring. See Section 8.1 for further information about results output.

The `ACTIVE PERIODS` command line determines when the torsional spring is active. See Section 2.5 for more information about this command line. Although the active periods option is available in the `TORSIONAL SPRING` command block, use of this option to turn the torsional spring off and on repeatedly is not recommended. Turning the torsional spring off and on repeatedly may lead to erroneous behavior in the spring model.
5.4 Mass Property Calculations

BEGIN MASS PROPERTIES
    # {block set commands}
    BLOCK = <string list>block_names
    INCLUDE ALL BLOCKS
    REMOVE BLOCK = <string list>block_names
    #
    # structure command
    STRUCTURE NAME = <string>structure_name
END [MASS PROPERTIES]

Presto automatically gives mass property information for the total model, which consists of all the
element blocks. (The mass for the total model, for example, is the total mass of all the element
blocks.) Presto also automatically gives mass property information for each element block.

In addition to the mass property information that is generated, Presto gives you the option of
defining a structure that represents some combination of element blocks and then of calculating
the mass properties for this particular structure. If you wish to define a structure that is a combination
of some group of element blocks, you must use the MASS PROPERTIES command block. This
command block appears in the region scope.

For the total model, each element block, and any user-defined structure, Presto reports the mass
and the center of mass in the global coordinate system. It also reports the moments and products
of inertia, as computed in the global coordinate system about the center of mass.

The MASS PROPERTIES command block contains two groups of commands—block set and struc-
ture. Each of these groups is basically independent of the other. Following are descriptions of the
two command groups.

5.4.1 Block Set Commands

The {block set commands} portion of the MASS PROPERTIES command block defines a set
of blocks for which mass properties are being requested, and can include some combination of the
following command lines:

    BLOCK = <string list>block_names
    INCLUDE ALL BLOCKS
    REMOVE BLOCK = <string list>block_names

These command lines, taken collectively, constitute a set of Boolean operators for constructing
a set of blocks. See Section 6.1.1 for more information about the use of these command lines
for creating a set of blocks used by the command block. There must be at least one BLOCK or
INCLUDE ALL BLOCKS command line in the command block.

The REMOVE BLOCK command line allows you to delete blocks from the set specified in the BLOCK
and/or INCLUDE ALL BLOCKS command line(s) through the string list block_names. Typically,
you will use the REMOVE BLOCK command line with the INCLUDE ALL BLOCKS command line. If you want to include all but a few of the element blocks, a combination of the REMOVE BLOCK command line and INCLUDE ALL BLOCKS should minimize input information.

Suppose that only one element block, block_300, is specified on the BLOCK command line. Then only the mass properties for that block will be calculated. If several element blocks are specified on the BLOCK command line, then that collection of blocks will be treated as one entity, and the mass properties for that single entity will be calculated. Thus, for example, if two element blocks, say, block_150 and block_210, are specified on the BLOCK command line, the total mass for the two element blocks will be reported as the total mass property.

5.4.2 Structure Command

The output for the mass properties will be identified by the command line:

```
STRUCTURE NAME = <string>structure_name
```

where the string structure_name is a user-defined name for the structure.
5.5 Element Death

BEGIN ELEMENT DEATH <string>death_name
# {block set commands}
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE BLOCK = <string list>block_names
#
# criteria commands
CRITERION IS AVG|MAX|MIN NODAL VALUE OF
 <string>var_name[(<integer>component_num)]
  |<=|=|>=| <real>tolerance
CRITERION IS ELEMENT VALUE OF
 <string>var_name[(<integer>component_num)]
  |<=|=|>=| <real>tolerance |
 <string>derived_quantity[(<integer>component_num)]
  |<=|=|>=| <real>tolerance
CRITERION IS GLOBAL VALUE OF
 <string>var_name[(<integer>component_num)]
  |<=|=|>=| <real>tolerance
ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
 = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
 = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
 = <string>param_value
MATERIAL CRITERION = <string list>material_model_names
#
# evaluation commands
CHECK STEP INTERVAL = <integer>num_steps
CHECK TIME INTERVAL = <real>delta_t
DEATH START TIME = <real>time
#
# miscellaneous option commands
DEATH ON INVERSION = OFF|ON(OFF)
DEATH STEPS = <integer>death_steps(1)
FORCE VALID ACME CONNECTIVITY
#
# additional command
ACTIVE PERIODS = <string list>period_names
END [ELEMENT DEATH <string>death_name]

The ELEMENT DEATH command block is used to remove elements from an analysis. For example, the command block can be used to remove elements that have fractured, that are no longer important to the analysis results, or that are nearing inversion. The name of the command block,
death_name, is user-defined and can be referenced in other commands to update boundary or contact conditions based on the death of elements creating new exposed surfaces.

Any element in an element block or element blocks selected in the ELEMENT DEATH command block is removed (killed) when one of the criteria specified in the ELEMENT DEATH command block is satisfied by that element. When an element dies, it is removed permanently. Any number of ELEMENT DEATH command blocks may exist within a region. However, a particular block of elements may be associated with at most one element death definition. If all of the elements in a region are killed, the analysis will terminate. If all of the elements attached to a node are killed, the mass for the node and all associated nodal quantities will be set to zero. If an element is killed, but an attached element is not, the mass of the killed element will remain at the nodes shared with the “living” element.

Elements may be killed using a derived stress, a derived strain, or a derived log strain quantity. To kill elements using a derived quantity, the quantity must be specifically listed in one of the command blocks described in Section 5.6.

The ELEMENT DEATH command block contains four groups of commands—block set, criteria, evaluation, and miscellaneous. In addition to the command lines in the four groups, there is one additional command line: ACTIVE PERIODS. The command block must contain commands from the block set and criteria groups. Command lines from the evaluation and miscellaneous groups are optional, as is the additional command. Following are descriptions of the different command groups and the ACTIVE PERIODS command line, an example of using the ELEMENT DEATH command block, and some concluding remarks related to element death visualization.

5.5.1 Block Set Commands

```
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE BLOCK = <string list>block_names
```

The block set commands portion of the ELEMENT DEATH command block defines a set of blocks for selecting the elements to be referenced. These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of blocks, as described in Section 6.1.1.

Element death must apply to a group of elements. There are two commands for selecting the elements to be referenced: BLOCK and INCLUDE ALL BLOCKS. In the BLOCK command line, you can list a series of blocks through the string list block_names. This command line may also be repeated multiple times. The INCLUDE ALL BLOCKS command line adds all the element blocks present in the region to the current element death definition. There must be at least one BLOCK or INCLUDE ALL BLOCKS command line in the ELEMENT DEATH command block.

The REMOVE BLOCK command line allows you to delete blocks from the set specified in the BLOCK and/or INCLUDE ALL BLOCKS command line(s) through the string list block_names. Typically, you will use the REMOVE BLOCK command line with the INCLUDE ALL BLOCKS command line. If you want to include all but a few of the element blocks, a combination of the REMOVE BLOCK command line and INCLUDE ALL BLOCKS command line should minimize input information.
5.5.2 Criteria Commands

Any combination of death criteria (CRITERION IS NODAL, CRITERION IS ELEMENT, CRITERION IS GLOBAL, ELEMENT BLOCK SUBROUTINE, MATERIAL CRITERION) can be specified within a single ELEMENT DEATH command block. However, only one user subroutine criterion may appear in a set of criteria command lines. As long as any one criterion is met, element death will occur. You do not have to meet all criteria that appear in an ELEMENT DEATH command block for element death to occur. Element death with multiple criteria is an OR condition rather than an AND condition.

A problem with a material that has both a tension cutoff and a compression cutoff would be an example for which you would want to use element death with multiple criteria. You would use one criterion to set failure in tension and another criterion to set failure in compression. If either the tension cutoff value, as set by the tension criterion, or the compression cutoff value, as set by the compression criterion, was exceeded for an element, the element would be killed.

As another example, you might have a problem that uses a nodal criterion and a user subroutine criterion. For this second example, you are precluded from using another subroutine criterion because you already have one. You could add some combination of nodal, element, global, or material criteria to the existing nodal and subroutine criteria, but you could not add another subroutine criterion.

5.5.2.1 Nodal Variable Death Criterion

\[
\text{CRITERION IS } \text{AVG}|\text{MAX}|\text{MIN NODAL VALUE OF} \\
\text{<string>}\text{var_name}\text{[(<integer>component_num)]} \\
\text{<|<=|=|>=|>|<} \text{<real>tolerance}
\]

Any registered Presto nodal variable may be used by an element death criterion, as specified in this nodal criterion command line.

The input parameters are described as follows:

- Nodal variables are present on the nodes of an element, and these nodal values must be reduced to a single element value for use by the criterion. The available types of reduction are AVG, which takes the average of the nodal values; MAX, which takes the maximum of the nodal values; and MIN, which takes the minimum of the nodal values.

- The string \text{var_name} gives the name of the registered variable. See Section 8.6 for a listing of the registered variables.

- For variables with multiple components, a component number can be specified. For example, a value of (2) for \text{component_num} refers to the \text{y} component of displacement. See Table 8.4 in Chapter 8 for how to determine the component number.

- The specified variable, with an optional component specification if the variable has components, may be compared to a given tolerance with one of five operators. The operator is
specified with the appropriate symbol for less than (\(<\)) less than or equal to (\(<\leq\)) equal to (\(=\)), greater than or equal to (\(\geq\)), or greater than (\(>\)). The given tolerance is specified with the real value \(tolerance\).

Any user-defined variable is also treated as a registered variable (see Section 9.2.4). Therefore, you could use a user-defined variable as the \(\text{var\_name}\) in the above death criterion command line, and the syntax will actually accept this usage of a user-defined variable. However, the use of a user-defined variable in a death criterion command line is not recommended. There are timing (when user-defined variables are calculated) and parallel issues regarding the use of a user-defined variable with element death. User subroutines should cover situations for element death where you might want to reference a user variable.

### 5.5.2.2 Element Variable Death Criterion

```
CRITERION IS ELEMENT VALUE OF 
<string>var_name[(<integer>component_num)] 
|<=|>=|> <real>tolerance 
<string>derived_quantity[(<integer>int_num)] 
|<=|>=|> <real>tolerance
```

Any registered Presto element variable, derived stress quantity, derived strain quantity, or derived log strain quantity may be used by an element death criterion, as specified in this element criterion command line. An element variable or a derived quantity is present on the element itself, so no reduction is required, which is why the first line in the format of the above command line differs from that of the nodal criterion command line in Section 5.5.2.1. As shown in the command line format above, the input parameters for an element variable differ somewhat from those of a derived quantity and are thus described separately.

**For a criterion using an element variable**, the variable name, component number, and tolerance can be specified in the same manner as defined for the nodal criterion command line.

The input parameters for the case of an element variable name are described as follows:

- The string \(\text{var\_name}\) gives the name of the registered variable. See Section 8.6 for a listing of the registered variables.

- For variables with multiple components, a component number can be specified. For example, a value of \(2\) for \(\text{component\_num}\) refers to the \(yy\) component of stress. See Table 8.4 in Chapter 8 for how to determine the component number.

- The specified variable, with an optional component specification if the variable has components, may be compared to a given tolerance with one of five operators. The operator is specified with the appropriate symbol for less than (\(<\)) less than or equal to (\(\leq\)), equal to (\(=\)), greater than or equal to (\(\geq\)), or greater than (\(>\)). The given tolerance is specified with the real value \(tolerance\).
Element state variables can also be used as criteria for element death. The syntax used to specify the variable name differs depending on the type of material model used.

- For default solid material models, the variable name is called out as:
  
  \[ \text{state}_{\text{material}}_{\text{name}}(\text{index}) \]

  where \text{material\_name} is the name of the material model, e.g. \text{elastic\_plastic}, and \text{index} is the index in the state variable array of the particular state variable to be used for the death criterion. For example, the command:
  
  \[ \text{criterion} = \text{element value of state}_{\text{elastic}}_{\text{plastic}}(1) > 0.9 \]

  uses the value of the first state variable for the elastic\_plastic material, which is the equivalent plastic strain. Note that the \text{MAT}\% syntax used for state variable output is \textit{not} used for element death based on state variables.

- For LAME solid material models, the variable name is called out directly by name.

- For shell material models, the variable name is called out directly by name. However, the name must be followed by an integer index in parentheses that denotes the integration point for the state variable. For example, the command:
  
  \[ \text{criterion} = \text{element value of crack}\_\text{opening}\_\text{strain}(1) > 0.01 \]

  would use the value of the state variable \text{crack\_opening\_strain} at the first integration point through the shell thickness in the criterion for element death.

Refer to Section 8.6.2 for tables with listings of state variables for the various material models.

Any user-defined variable is also treated as a registered variable (see Section 9.2.4). Therefore, you could use a user-defined variable as the \text{var\_name} in the above death criterion command line, and the syntax will actually accept this usage of a user-defined variable. However, the use of a user-defined variable in a death criterion command line is not recommended. There are timing (when user-defined variables are calculated) and parallel issues regarding the use of a user-defined variable with element death. User subroutines should cover situations for element death where you might want to reference a user variable.

For a criterion using a derived quantity, the derived quantity name, integration point number, and tolerance can be specified. The complete set of derived stress, strain, and log strain quantities is described in Section 8.1.1.4, which deals with the output of derived quantities. Table 8.1 lists all derived stress quantities, Table 8.3 lists all derived strain quantities, and Table 8.2 lists all derived log strain quantities.

The input parameters for the case of a derived quantity are described as follows:

- The string \text{derived\_quantity} gives the name of the derived quantity. See Section 8.1.1.4 for a listing of the derived quantities.

- For a derived quantity defined at multiple integration points, an integration point number can be specified. The parameter \text{int\_num} specifies the integration point for the derived
quantity. For example, if you wanted to use the von Mises stress at integration point 3 for an element criterion, you would use `von_mises` for `derived_quantity` and `(3)` for `int_num`, which would appear as follows:

CRITERION IS ELEMENT VALUE OF von_mises(3)

- The specified variable, with an optional component specification if the variable has components, may be compared to a given tolerance with one of five operators. The operator is specified with the appropriate symbol for less than (`<`), less than or equal to (`<=`), equal to (`=`), greater than or equal to (`>=`), or greater than (`>`). The given tolerance is specified with the real value `tolerance`.

Importantly, when you specify a derived quantity via the `CRITERION IS ELEMENT VALUE OF` command line, you may also need to include an associated command block for the specific quantity. The associated command block for a derived stress is `DERIVED OUTPUT`; for a derived strain, it is `DERIVED STRAIN OUTPUT`; and for a derived log strain, it is `DERIVED LOG STRAIN OUTPUT`. These three command blocks are described in Section 5.6. The conditions determining their usage are partly contingent upon certain output considerations and are discussed next.

As explained in Section 8.1.1.4, derived quantities can be output in the results file using the `ELEMENT VARIABLES` command line. If you specify the derived quantity that you want to use as a criterion for element death in the `ELEMENT VARIABLES` command line in the `RESULTS OUTPUT` command block, you do not need to include the command block in Section 5.6 associated with that derived quantity because Presto will calculate the derived quantity for output and make it available for use as an element death criterion. However, if you only want to use the derived quantity as a criterion for element death and you do not want to have it calculated for output, you will need to include the associated command block (`DERIVED OUTPUT`, `DERIVED STRAIN OUTPUT`, or `DERIVED LOG STRAIN OUTPUT`) for the particular derived quantity in the input file.

### 5.5.2.3 Global Death Criterion

CRITERION IS GLOBAL VALUE OF

<string>var_name[(<integer>component_num)]

<|<=|=|>=|> <real>tolerance

Any registered Presto global variable may be used as an element death criterion. Once the global criterion is reached, all elements specified in the `ELEMENT DEATH` command block are killed. The variable name, component number, and tolerance can be specified in the same manner as defined for the nodal criterion command line.

The input parameters are described as follows:

- The string `var_name` gives the name of the registered variable. See Section 8.6 for a listing of the registered variables.
- For variables with multiple components, a component number can be attached. Global variables are typically scalar quantities. If you encounter a global variable with multiple components, consult with Table 8.4 in Chapter 8 for how to determine the component number. Section 5.5.2.1 and Section 5.5.2.2 provide examples of using the component option.

- The specified variable, with an optional component specification if the variable has components, may be compared to a given tolerance with one of five operators. The operator is specified with the appropriate symbol for less than (\(<\)), less than or equal to (\(<=\)), equal to (\(=\)), greater than or equal to (\(>=\)), or greater than (\(>\)). The given tolerance is specified with the real value tolerance.

5.5.2.4 Subroutine Death Criterion

```
ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
```

A death criterion can be specified via a user-defined subroutine (see Chapter 9), which is invoked by the ELEMENT BLOCK SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user. The user-defined subroutine for element death must be an element subroutine signature (see Section 9.2.2). The element subroutine will return an output values array and a flag array of one flag per element (see Table 9.2 in Chapter 9). The output values array is ignored. Death is determined by the flag return value. For user-defined subroutines, a flag return value of –1 indicates that the element should die. A flag return value greater than or equal to 0 indicates that the element should remain alive.

Following the ELEMENT BLOCK SUBROUTINE command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 9.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided throughout Section 9.

5.5.2.5 Material Death Criterion

```
MATERIAL CRITERION = <string list>material_model_names
```

Some material models have a failure criterion. When this failure criterion is satisfied within an element, the element has fractured or disintegrated. The material models reduce the stress in these fractured or disintegrated elements to zero. The MATERIAL CRITERION command line can be used to remove these fractured or disintegrated elements from an analysis. Removal of the
fractured elements will speed computations, enhance visualization, and prevent spurious inversion of these elements that may stop the analysis.

The current supported material models for use by the `MATERIAL CRITERION` command line are `ELASTIC_FRACTURE` (see Section 4.2.2), `DUCTILE_FRACTURE` (see Section 4.2.5), and `ML_EP_FAIL` (see Section 4.2.7). Note that `MATERIAL CRITERION` support for the `ML_EP_FAIL` model is only supported for solid elements; though the `ML_EP_FAIL` model is available for shells, the `MATERIAL CRITERION` does not yet support them. Instead, kill the shell element when the state variable `CRACK_OPENING_STRAIN` reaches or exceeds the value specified in the input deck for that material.

Suppose you have an element block named `part1_ss304` that references a material named `SS304`. This material, `SS304`, uses the `DUCTILE_FRACTURE` material model (see Section 4.2.5). You also have an element block named `ring5_al6061` that references a material named `al6061`. This material, `al6061`, uses the `ML_EP_FAIL` material model (see Section 4.2.7). If you have an `ELEMENT DEATH` command block with the command line:

```
BLOCK = part1_ss304 ring5_al6061
```

and the command line:

```
MATERIAL CRITERION = DUCTILE_FRACTURE ML_EP_FAIL
```

then any element in `part1_ss304` that fails according to the material model `DUCTILE_FRACTURE` (in material `SS304`) and any element in `ring5_al6061` that fails according to the material model `ML_EP_FAIL` (in material `al6061`) will be killed by element death.

### 5.5.3 Evaluation Commands

- `CHECK STEP INTERVAL = <integer>num_steps`
- `CHECK TIME INTERVAL = <real>delta_t`
- `DEATH START TIME = <real>time`

Evaluation of element death criteria may be time consuming. Additionally, reconstruction of contact or other boundary conditions after element death can be very time consuming. For these reasons, three command lines are available for determining the frequency at which element death is evaluated. The default is to evaluate element death at every time step. You can limit the number of times at which the element death evaluation is done by using the following commands.

- The `CHECK STEP INTERVAL` command line instructs element death to evaluate the element death criteria only every `num_steps` time steps.
- The `CHECK TIME INTERVAL` command line instructs element death to evaluate the element death criteria only every `delta_t` time units.
- The `DEATH START TIME` command line instructs element death not to evaluate death criteria before a user-specified time, as given by the real value `time`. 
You may use both the `CHECK STEP INTERVAL` and `CHECK TIME INTERVAL` command lines in a command block. Evaluations for element death will be made at both the time and step intervals if both of these command lines are included.

All three of the above command lines—`CHECK STEP INTERVAL`, `CHECK TIME INTERVAL`, and `DEATH START TIME`—are optional command lines.

### 5.5.4 Miscellaneous Option Commands

The command lines listed below need not be present in the `ELEMENT DEATH` command block unless the conditions addressed by each call for their inclusion.

#### 5.5.4.1 Death on Inversion

```
DEATH ON INVERSION = ON|OFF(OFF)
```

If the `DEATH ON INVERSION` command line is on, any element that inverts will be killed. This command only works for uniform gradient 8-noded hex elements and 4-, 8-, and 10-noded tet elements.

#### 5.5.4.2 Death Steps

```
DEATH STEPS = <integer>death_steps(1)
```

If the `DEATH STEPS` command line is used and the value for `death_steps` is set to some value greater than 1, the stress in a killed element will not be set to 0 until the prescribed number of steps has occurred. The stress in the killed element will decrease (if it is positive) to 0 in a linear fashion over the prescribed number of steps; the stress in the killed element will increase (if it is negative) to 0 over the prescribed number of steps. If the stress in a killed element is set to 0 over a single time step, the resulting change in stress can sometimes cause instabilities due to the sudden release of energy. However, elimination of the stress over an excessive number of load steps can make it appear as if the element is present long after it has been killed. The default number of steps, as provided in the integer value `death_steps`, is 1.

The value you select for `death_steps` will depend on your analysis. A small number such as 3 or 5 may be sufficient to prevent instabilities for most cases. However, in some cases it may be necessary to use a value for `death_steps` of 10 or larger. The loads, material models, and model complexity in your analysis will impact the value of `death_steps`.

#### 5.5.4.3 Degenerate Mesh Repair

```
FORCE VALID ACME CONNECTIVITY
```
If the FORCE VALID ACME CONNECTIVITY command line is present, degenerate mesh occurrences will be repaired. Element death has the possibility of creating degenerate mesh occurrences that will not be accepted by the ACME (see Reference 12) contact algorithms used by Presto. For example, if two continuum elements are connected only by an edge, ACME will not accept the mesh as a valid mesh. For this degenerate mesh occurrence (continuum elements connected only at an edge), the degeneracy is repaired by deleting all elements attached to the offending edge if we have turned on this repair option.

The option to repair degenerate mesh occurrences is on by default if there is a CONTACT DEFINITION command block that includes the command line:

```
UPDATE ALL SURFACES FOR ELEMENT DEATH = ON
```

See Section 7.4 for a full description of the UPDATE ALL SURFACES FOR ELEMENT DEATH command line.

If you do not have a CONTACT DEFINITION command block and want to repair degenerate mesh occurrences for whatever purposes, you should include the FORCE VALID ACME CONNECTIVITY command line.

### 5.5.4.4 Additional Command

The ACTIVE PERIODS command line can appear as an option in the ELEMENT DEATH command block:

```
ACTIVE PERIODS = <string list>period_names
```

This command line determines when element death is active. See Section 2.5 for more information about this optional command line.

### 5.5.5 Example

The following example provides instructions to kill elements in block_1 when they leave a bounding box. This type of element death can be useful in an analysis where some peripheral parts, because of fracture, separate and fly away from a central body, this central body being our part of interest. In this case, these peripheral parts no longer impact the solution. The instructions in this ELEMENT DEATH command block will cause the parts to be killed, thus speeding up the computation.

```
begin element death out_of_bounds
  block = block_1
  # check x coordinates
  criterion is avg nodal value of coordinates(1) >= 10
  criterion is avg nodal value of coordinates(1) <= -10
  # check y coordinates
  criterion is avg nodal value of coordinates(2) >= 10
  criterion is avg nodal value of coordinates(2) <= -10
end element death
```
# check z coordinates
criterion is avg nodal value of coordinates(3) >= 10
criterion is avg nodal value of coordinates(3) <= -10
end element death out_of_bounds

## 5.5.6 Element Death Visualization

When an element dies, information about this element will still be sent, along with information for all other elements, to the Exodus II results file. (Chapter 8 describes the output of element variables to the results file.) The death status of the elements may be output to the results file by requesting element variable output for the element variable DEATH_DUMMY_VAR. Including the command line

```
ELEMENT VARIABLES = DEATH_DUMMY_VAR as death_var
```

in a RESULTS OUTPUT command block (Chapter 8) will output this element variable with the name death_var in the results file.

The convention for DEATH_DUMMY_VAR is as follows: An element with a value of 1.0 for DEATH_DUMMY_VAR is a living element. An element with a value of 0.0 for DEATH_DUMMY_VAR is a dead element. A value less than 0.0 indicates that the element was killed due to a code related issue (e.g. an unsupported geometry issue related to ACME). A value between 1.0 and 0.0 indicates an element in the process of dying. A dying element has its material stress scaled down over a number of time steps. The current scaling factor for an element is given by DEATH_DUMMY_VAR. Whether or not an element can have a value for DEATH_DUMMY_VAR other than 0.0 or 1.0 will depend on whether or not you have used the DEATH STEPS option in the ELEMENT DEATH command block. If the number of steps over which death occurs is greater than 1, then DEATH_DUMMY_VAR can be some value between 0.0 and 1.0.

If DEATH_DUMMY_VAR is written to a results file, and the results file is used in some visualization program to examine the mesh for the model, it is possible to use DEATH_DUMMY_VAR to exclude killed elements in any view of the model. A subset of the mesh showing just the living elements can be created by selecting only those elements with DEATH_DUMMY_VAR = 1.0 values.
5.6 Derived Quantities for Element Death

The above command blocks are used in conjunction with the CRITERION IS ELEMENT VALUE OF command line in the ELEMENT DEATH command block (see Section 5.5.2.2). Each of the blocks is associated with a type of derived quantity: DERIVED OUTPUT is associated with derived stress, DERIVED STRAIN OUTPUT with derived strain, and DERIVED LOG STRAIN OUTPUT with derived log strain. Structured similarly, each of the three command blocks can contain one or more command lines, with each command line requiring a single value, the string derived_quantity_name. The derived quantity specified by derived_quantity_name will also appear on a CRITERION IS ELEMENT VALUE command line. If a derived quantity is referenced on a CRITERION IS ELEMENT VALUE command line, it must appear in one of the above three command blocks unless the condition described in the following paragraph is satisfied.

As discussed in Section 5.5.2.2, the inclusion of one of the three command blocks above is not mandatory when you have specified the desired quantity in a CRITERION IS ELEMENT VALUE command line. You only need to specify the applicable command block for the derived quantity if you have not specified that same derived quantity for output in the RESULTS OUTPUT file via the ELEMENT VARIABLES command line.

Following are some examples of using the three command blocks discussed in this section.

- If you want to use a derived stress quantity for an element death option (and not for output), you must include a DERIVED OUTPUT command block. Suppose you want an element death option that uses the von Mises stress, then you would include the following command block:

BEGIN DERIVED OUTPUT
  COMPUTE AND STORE STRESS VARIABLE = von_mises
END DERIVED OUTPUT

Consult Table 8.1 for a complete listing of derived stress quantities.
If you want to use a derived strain quantity for an element death option (and not for output), you must include a `DERIVED STRAIN OUTPUT` command block. Suppose you want an element death option using the octahedral shear strain (see Section 8.1.1.4). Then you would include the following command block:

```
BEGIN DERIVED STRAIN OUTPUT
  COMPUTE AND STORE STRAIN VARIABLE = octahedral_shear_strain
END DERIVED STRAIN OUTPUT
```

Consult Table 8.3 for a complete listing of derived strain quantities.

If you want to use a derived log strain quantity for an element death option (and not for output), you must include a `DERIVED LOG STRAIN OUTPUT` command block. Suppose you want element death options using the octahedral shear log strain and the first invariant of the log strain (see Section 8.1.1.4). Then you would include the following command block:

```
BEGIN DERIVED LOG STRAIN OUTPUT
  COMPUTE AND STORE LOG STRAIN VARIABLE = octahedral_shear_log_strain
  COMPUTE AND STORE LOG STRAIN VARIABLE = log_stain_invariant_1
END DERIVED LOG STRAIN OUTPUT
```

The above example would require that two `CRITERION FOR ELEMENT VALUE OF` command lines be included in the `ELEMENT DEATH` command block, one providing the criterion for `octahedral_shear_log_strain` and the other providing the criterion for `octahedral_shear_log_strain`. Consult Table 8.2 for a complete listing of derived log strain quantities.
5.7 Mesh Rebalancing

Mesh rebalancing is a feature in Presto that may improve the efficiency of an analysis. Two command blocks can be used to control mesh rebalancing: REBALANCE and ZOLTAN PARAMETERS. The REBALANCE command block is required; the ZOLTAN PARAMETERS command block is optional. Sections 5.7.1 and 5.7.2 describe these command blocks.

5.7.1 Rebalance

BEGIN REBALANCE
  INITIAL REBALANCE = ON|OFF (OFF)
  PERIODIC REBALANCE = ON|OFF|AUTO (OFF)
  STEP INTERVAL = <integer>step_interval
  COMMUNICATION RATIO THRESHOLD = <real>ratio
  ZOLTAN PARAMETERS = <string>parameter_name
END REBALANCE

Initial decomposition of a mesh for parallel runs with Presto is done by a utility called loadbal. The initial decomposition provided by loadbal may not provide a decomposition for good-to-optimal parallel performance of Presto under certain circumstances. Therefore, Presto supports a simple mesh-rebalancing capability that can be used to improve the parallel performance of some problems. When mesh rebalancing is invoked, the parallel decomposition is changed, and elements are moved among the processors to balance the computational load and minimize the processor-to-processor communication. Mesh rebalancing may be useful in the following circumstances:

- The mesh decomposition produced by loadbal for SPH meshes is nearly always poor. It is recommended that an initial mesh rebalance be done for all SPH problems.

- If a problem experiences very large deformations, periodic rebalancing may be helpful. In contact or SPH problems, communication is performed between physically nearby contact surfaces or SPH particles. To maintain optimum performance, it is helpful to have neighboring particles located on the same processors. Periodic mesh rebalancing can ensure that neighboring entities tend to remain on the same processor during large mesh deformations.

The REBALANCE command block is placed in the Presto region scope. The mesh rebalancing in Presto uses a mesh balancing library called Zoltan (Reference [3]). Zoltan performs the actual rebalancing. By default, Presto creates a Zoltan object with a default set of parameters. However, a Zoltan object with a customized set of parameters can be created and referenced from the REBALANCE command block.

5.7.1.1 Rebalance Command Lines

INITIAL REBALANCE = on|off (off)
PERIODIC REBALANCE = on|off|auto (off)
STEP INTERVAL = <integer>step_interval
COMMUNICATION RATIO THRESHOLD = <real>ratio

The above command lines control the frequency at which the rebalancing is done.

The INITIAL REBALANCE command line is used to rebalance the mesh at time zero before any calculations occur. This option should be used if the initial mesh decomposition passed to Presto is poor.

If the PERIODIC REBALANCE command option is on, the mesh will be rebalanced every step interval steps, where step_interval is the parameter specified by the STEP INTERVAL command line. If the option is auto, the mesh will be rebalanced every step_interval steps or when the communication ratio reaches a critical value. The communication ratio is currently defined only for SPH problems. The communication ratio is a measure of how much communication is required in the current mesh decomposition versus an estimate of what the communication could be with an optimal decomposition. Mesh rebalancing is expensive, so rebalancing should be done rarely. The communication ratio is set by the parameter ratio on the COMMUNICATION RATIO THRESHOLD command line. A communication ratio parameter in the range of 1.25 to 1.5 is usually ideal.

5.7.1.2 Zoltan Command Line

The command line

    ZOLTAN PARAMETERS = <string>parameter_name

references a ZOLTAN PARAMETERS command block named parameter_name. Various parameters for Zoltan can be set in the ZOLTAN PARAMETERS command block. If you do not use the ZOLTAN PARAMETERS command line, a default set of parameters is used. The default parameter command block is shown as follows:

    BEGIN ZOLTAN PARAMETERS default
    LOAD BALANCING METHOD = recursive coordinate bisection
    # string parameter
    OVER ALLOCATE MEMORY = 1.5 # real parameter
    REUSE CUTS = true # string parameter
    ALGORITHM DEBUG LEVEL = 0 # integer parameter
    CHECK GEOMETRY = true # string parameter
    ZOLTAN DEBUG LEVEL = 0 # integer parameter
    END ZOLTAN PARAMETERS default

See Section 5.7.2 for a discussion of the ZOLTAN PARAMETERS command block. Section 5.7.2 lists the command lines that can be used to set Zoltan parameters.
5.7. MESH REBALANCING

5.7.2 Zoltan Parameters

BEGIN ZOLTAN PARAMETERS <string>parameter_name
  LOAD BALANCING METHOD = <string>recursive coordinate bisection|
  recursive inertial bisection|hilbert space filling curve|
  octree
  DETERMINISTIC DECOMPOSITION = <string>false|true
  IMBALANCE TOLERANCE = <real>imb_tol
  OVER ALLOCATE MEMORY = <real>over_all_mem
  REUSE CUTS = <string>false|true
  ALGORITHM DEBUG LEVEL = <integer>alg_level
    # 0<=(alg_level)<=3
  CHECK GEOMETRY = <string>false|true
  KEEP CUTS = <string>false|true
  LOCK RCB DIRECTIONS = <string>false|true
  SET RCB DIRECTIONS = <string>do not order cuts|xyz|xzy|
  yxz|yxz|zxy
  RECTILINEAR RCB BLOCKS = <string>false|true
  RENUMBER PARTITIONS = <string>false|true
  OCTREE DIMENSION = <integer>oct_dimension
  OCTREE METHOD = <string>morton indexing|grey code|hilbert
  OCTREE MIN OBJECTS = <integer>min_obj # 1<=(min_obj)
  OCTREE MAX OBJECTS = <integer>max_obj # 1<=(max_obj)
  ZOLTAN DEBUG LEVEL = <integer>zoltan_level
    # 0<=(zoltan_level)<=10
  DEBUG PROCESSOR NUMBER = <integer>proc # 1<=proc
  TIMER = <string> wall|cpu
  DEBUG MEMORY = <integer>dbg_mem # 0<=(dbg_mem)<=3
END [ZOLTAN PARAMETERS <string>parameter_name]

The ZOLTAN PARAMETERS command block is used to set parameters for Zoltan (see Reference 13), a program that can be used for mesh rebalancing in Presto. The ZOLTAN PARAMETERS command block is used in association with the REBALANCE command block. A REBALANCE command block may reference a ZOLTAN PARAMETERS command block via the name, parameter_name, for the parameter command block. Reference Section 5.7.1 regarding the use of the ZOLTAN PARAMETERS command block for mesh rebalancing in Presto.

Setting the parameters for Zoltan involves some understanding of how Zoltan works. We will not present a discussion of the various parameters that you may set in the ZOLTAN PARAMETERS command block. You should consult with Reference 13 for a discussion of the parameters that can be set by the various command lines in the ZOLTAN PARAMETERS command block. Note that some of the command lines in this command block have comments that provide additional information about the parameters. The “\#” symbol precedes a comment.

In the above command block, = and IS are the allowed delimiters, which is different from the usual Presto convention of =, IS, and ARE. Note that the ZOLTAN PARAMETERS command block should be specified in the domain scope when it is referenced from the ZOLTAN PARAMETERS command line in the REBALANCE command block. When the default set of parameters is used for
a Zoltan object, the ZOLTAN PARAMETERS command block need not be included in the input file.

### 5.8 References


Chapter 6

Boundary Conditions and Initial Conditions

Presto offers a variety of options for defining boundary and initial conditions. Typically, boundary and initial conditions are defined on some subset of mesh entities (node, element face, element) defining a model. Presto offers a flexible means to define subsets of mesh entities. Section 6.1.1 describes commands that will let you define some subset of a mesh entity using a collection of commands that constitute a set of Boolean operators.

The remaining parts of this chapter discuss the following functionality:

- Section 6.2 presents methods for setting the initial values of registered variables in Presto. Presto has the flexibility to set a complex initial state for some variable such as nodal velocity or element stress.

- Kinematic boundary conditions typical of those you would expect in an explicit, transient dynamics code (fixed displacement, prescribed acceleration, etc.) are options in Presto and described in Section 6.3. Most of these boundary conditions let you specify a time history using some SIERRA function or a more complex time-varying and spatially varying history with a user subroutine.

- Section 6.4 documents a number of initial velocity options available in Presto.

- Force boundary conditions typical of those you would expect in an explicit, transient dynamics code (prescribed force, traction, etc.) are options in Presto and described in Section 6.5. Most of these force boundary conditions let you specify a time history using some SIERRA function or a more complex time-varying and spatially varying history with a user subroutine.

- Section 6.6 discusses the gravity load option. A gravity load is a body force boundary condition.

- Section 6.7 details a number of options available for describing a temperature field in Presto.

- Presto has a number of specialized boundary conditions—cavity expansion, silent boundary, spot-weld, and line weld. These specialized boundary conditions are described in Section 6.8.
6.1 General Boundary Condition Concepts

There are general principles that apply to all of the available types of boundary conditions. To apply a boundary condition, a set of mesh entities and the magnitude and/or direction in which it is to be applied must be specified. Presto provides several methods for both specifying the set of mesh entities and for prescribing how the boundary condition is to be applied. The general concepts on how this is done are applicable to all of the boundary condition types, and are described in the following sections.

6.1.1 Mesh-Entity Assignment Commands

A number of standard command lines exist to define a set of mesh entities (node, element face, element) associated with some type of mechanics. (Mechanics can be a boundary condition, an initial condition, or a gravity load.) All these command lines exist within the command blocks for the various mechanics, which in turn exist within the region scope. These command lines, taken collectively, constitute a set of boolean operators for constructing sets of mesh entities.

The first set of command lines we will consider is as follows:

\[
\begin{align*}
\text{NODE SET} &= \text{<string list>} \text{nodelist_names} \\
\text{SURFACE} &= \text{<string list>} \text{surface_names} \\
\text{BLOCK} &= \text{<string list>} \text{block_names} \\
\text{INCLUDE} &= \text{ ALL BLOCKS}
\end{align*}
\]

In the above command lines, the string list \text{nodelist_names} is used to represent one or more node sets as discussed in Section 1.5. A node set is referenced as \text{nodelist_id}, where id is some integer. For example, suppose you have three node lists in your model: 10, 23, and 105. If you want to combine all these node lists so that they form one set of nodes for, say, your boundary condition or initial condition, then you would use the command line:

\[
\text{NODE SET} = \text{nodelist}_10 \text{ nodelist}_23 \text{ nodelist}_105
\]

This convention applies as well to any surface-related command line that uses the string list \text{surface_names} or any block-related command line that uses the string list \text{block_names}.

The \text{NODE SET} command line associates a set of nodes with a mechanics. A mechanics may be applied to multiple node sets by putting multiple node set names on the command line or by repeating the command line multiple times.

The \text{SURFACE} command line associates a set of element faces with a mechanics. A mechanics may be applied to multiple surfaces by putting multiple surface names on the command line or by repeating the command line multiple times. The \text{SURFACE} command line can also be used to associate a set of nodes with a mechanics. For example, suppose we wish to use the fixed displacement kinematic boundary condition. Although this is a nodal boundary condition (the condition is applied to individual nodes), a \text{SURFACE} command line can be used to establish the set of nodes. If the command line
SURFACE = surface_101

appears in a fixed displacement boundary condition, then all the nodes associated with surface 101 will be associated with the boundary condition.

The BLOCK command line associates a set of elements with a mechanics. A mechanics may be applied to multiple blocks by putting multiple block names on the command line or by repeating the command line multiple times. The BLOCK command line can also be used to associate a set of nodes with a mechanics. For example, suppose we wish to use the fixed displacement kinematic boundary condition as in the previous example. If the command line

   BLOCK = block_50

appears in a fixed displacement kinematic boundary condition, then all the nodes associated with block 50 will be associated with the boundary condition.

The INCLUDE ALL BLOCKS command line associates all blocks with a mechanics. This will apply the mechanics to all nodes and elements in the model.

The block-related command lines associated with contact will generate surfaces. The block command lines associated with boundary conditions, initial conditions, and gravity will NOT generate surfaces.

Any combination of the above command lines can be used to create a union of mesh entities. Suppose, for example, that the command lines

   NODE SET = nodelist_2
   SURFACE = surface_3

appear in a FIXED DISPLACEMENT command block for a kinematic boundary condition. The set of nodes associated with the boundary condition will be the union of the set of nodes associated with surface 3 and the set of nodes associated with node set 2.

When a union of mesh entities is created by using two or more of the above command lines, a mesh entity may appear in more than one topological entity—node set, surface, block. However, the mechanics is applied to the mesh entity only once. For example, node 67 may be a part of nodelist 2 and surface 3. Including both nodelist 2 and surface 3 into a mechanics will only apply the mechanics to node 67 once.

The set of mesh entities associated with a mechanics can be edited (mesh entities can be deleted from the set) by using the following command lines:

   REMOVE NODE SET = <string list>nodelist_names
   REMOVE SURFACE = <string list>surface_names
   REMOVE BLOCK = <string list>block_names

The REMOVE NODE SET command line deletes a set of nodes from the node set associated with a mechanics.

The REMOVE SURFACE command line deletes a set of element faces from the set of element faces associated with a mechanics. It will remove a set of nodes associated with the surface from the set of nodes associated with the mechanics.
The `REMOVE BLOCK` command line deletes a set of elements from the set of elements associated with a mechanics. It will remove a set of nodes associated with the block from the node set associated with the mechanics.

### 6.1.2 Methods for Specifying Boundary Conditions

There are three main methods which can be used to prescribe most types of boundary conditions available in Presto.

- The boundary condition can be prescribed using commands in the input file. These commands are categorized as “specification commands” in this document. Depending on the type of the boundary condition, it is be necessary to prescribe its direction and/or magnitude. Boundary conditions can be specified this way when a set of mesh entities is to experience a similar condition with a time variation that can be expressed by a function. One of the following commands is used to specify the direction of the boundary condition: `COMPONENT`, `DIRECTION`, `CYLINDRICAL AXIS`, or `RADIAL AXIS`. The magnitude is defined using one of `MAGNITUDE`, `FUNCTION` or `ANGULAR VELOCITY`. These commands are used in various combinations depending on the type of the boundary condition. The details of how to use them are provided in the descriptions of the various boundary condition types.

- If the nature of the boundary condition is such its variation in time and space can not be described easily by the combination of a function and a direction, it may be necessary to use a user-defined subroutine. User subroutines provide a very general capability to define how kinematic or force boundary conditions are applied. The use of user-defined subroutines does increase the complexity of defining the model, however. The user must write and debug the subroutine and compile and link it in with Presto. Because of the added complexity, user subroutines should only be used if the needed capability is not provided by the other methods of prescribing boundary conditions.

- For some types of boundary conditions, the values of the field to be prescribed can be read in from an existing output database. This is often used as a method to transfer results from one analysis code to another. One of the common uses for this capability is to compute temperatures using a thermal code, and then transfer the temperature fields to Presto to study combined mechanical and thermal effects. This capability can be used either to read in initial values or to read in a series of values that vary over time.

In the following sections describing specific types of boundary conditions, the commands are grouped according to these three categories.
6.2 Initial Variable Assignment

BEGIN INITIAL CONDITION
    # {mesh-entity set commands}
    NODE SET = <string list>node_list_names
    SURFACE = <string list>surface_names
    BLOCK = <string list>block_names
    INCLUDE ALL BLOCKS
    REMOVE NODE SET = <string list>node_list_names
    REMOVE SURFACE = <string list>surface_names
    REMOVE BLOCK = <string list>block_names
    #
    # variable identification commands
    INITIALIZE VARIABLE NAME = <string>var_name
    VARIABLE TYPE = [NODE|EDGE|FACE|ELEMENT|GLOBAL]
    #
    # specification command
    MAGNITUDE = <real list>initial_values
    #
    # input mesh commands
    READ VARIABLE = <string>mesh_var_name
    TIME = <real>time
    #
    # user subroutine commands
    NODE SET SUBROUTINE = <string>subroutine_name | 
    SURFACE SUBROUTINE = <string>subroutine_name | 
    ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
    SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
    SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
    SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
    SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
    #
    # additional command
    SCALE FACTOR = <real>scale_factor(1.0)
END [INITIAL CONDITION]

Presto supports a general initialization procedure for setting the value of any variable. This procedure can be used to set material state variables, shell thickness, initial stress, etc. There is minimal checking in Presto, however, to ensure that the changes made yield a consistent system. There is also no guarantee that the changes will not be overwritten or misinterpreted by some other internal routine depending on what variable is being changed. Thus, caution is advised when using this capability.
The **INITIAL CONDITION** command block, which appears in the region scope, is used to select a method and set values for initializing a variable. The command block specifies the initial value of a global variable or a variable associated with a set of mesh entities, i.e., nodes, edges, faces, or elements. The user has three options for setting initial values: with a constant magnitude, with an input mesh variable, or by a user subroutine. Only one of these three options can be specified in the command block.

The command block contains five groups of commands—mesh-entity set, variable identification, magnitude, input mesh variable, and user subroutine. In addition to the command lines in the five groups, there is one additional command line: **SCALE FACTOR**. Following are descriptions of the different command groups and the **SCALE FACTOR** command line.

### 6.2.1 Mesh-Entity Set Commands

The (mesh-entity set commands) portion of the **INITIAL CONDITION** command block specifies the nodes, element faces, or elements associated with the variable to be initialized. This portion of the command block can include some combination of the following command lines:

- **NODE SET = <string list>nodelist_names**
- **SURFACE = <string list>surface_names**
- **BLOCK = <string list>block_names**
- **INCLUDE ALL BLOCKS**
- **REMOVE NODE SET = <string list>nodelist_names**
- **REMOVE SURFACE = <string list>surface_names**
- **REMOVE BLOCK = <string list>block_names**

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes, element faces, or elements. See Section 6.1.1 for more information about the use of these command lines for mesh entities. There must be at least one **NODE SET, SURFACE, BLOCK, or INCLUDE ALL BLOCKS** command line in the command block.

### 6.2.2 Variable Identification Commands

Any variable used in the **INITIAL CONDITION** command block must exist in Presto. The variable can be any currently registered variable in Presto or any user-defined variable created with the **USER VARIABLE** command block (see Section 9.2.4).

There are two command lines that identify the variable:

- **INITIALIZE VARIABLE NAME = <string>var_name**
- **VARIABLE TYPE = [NODE|EDGE|FACE|ELEMENT|GLOBAL]**

The **INITIALIZE VARIABLE NAME** command line gives the name of the variable for which initial values are being assigned. As mentioned, the string **var_name** must be some variable known to Presto; it cannot be an arbitrary user-selected name.
6.2. INITIAL VARIABLE ASSIGNMENT

The VARIABLE TYPE command line provides additional information about the variable being initialized. The options NODE, EDGE, FACE, ELEMENT, and GLOBAL on the command line indicate whether the variable is, respectively, a nodal, edge, face, element, or global quantity. One of these options must appear in the VARIABLE TYPE command line.

Both of these command lines are required regardless of the option selected to set values for the variable.

6.2.3 Specification Command

If the constant magnitude command is used, one or more initial values are specified directly in the command block. This is done using the following command line:

```
MAGNITUDE = <real list>initial_values
```

The initial_values specified on the MAGNITUDE command line will set the values for the variable given by var_name in the INITIALIZE VARIABLE NAME command line. The number of values is dependent on the type of the variable specified in the INITIALIZE VARIABLE NAME command line. For example, if the user wanted to initialize the velocity at a set of nodes, three quantities would have to be specified since the velocity at a node is a vector quantity. If the user wanted to initialize the stress tensor for a set of uniform-gradient, eight-node hexahedral elements, six quantities would have to be specified since the stress tensor for this element type is described with six values.

6.2.4 Input Mesh Command

If the input mesh option is used, the initial values will be read from a variable that exists in a mesh file. As an example, suppose the mesh file contains a set of element temperatures. These temperature values (which can vary for each element) can be used to initialize a temperature value associated with each element.

Following are the command lines related to the input mesh option:

```
READ VARIABLE = <string>mesh_var_name
TIME = <real>temp_time
```

The string mesh_var_name must match the name of the variable in the mesh file. The number of values associated with the variable in the mesh file must be the same number associated with the variable name specified in the INITIALIZE VARIABLE NAME command line. For example, if the variable specified by the INITIALIZE VARIABLE NAME has a single value, then the variable specified in the mesh file must also have a single value. You may select the variable at a specific time by using the TIME command line. If the specified time on the TIME command line does not correspond exactly to a time on the mesh file, the data on the mesh file will be interpolated as needed to obtain the initial values.

The variable name used on the mesh file can be arbitrary. The name can be identical to or different from the registered variable name specified on the INITIALIZE VARIABLE NAME command line.
6.2.5 User Subroutine Commands

If the user subroutine option is used, the initial values will be calculated by a subroutine that is
written by the user explicitly for this purpose. The subroutine will be called by Presto at the
appropriate time to perform the calculations.

Following are the command lines related to the user subroutine option:

NODE SET SUBROUTINE = <string>subroutine_name |
SURFACE SUBROUTINE = <string>subroutine_name |
ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
   = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
   = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
   = <string>param_value

Only one of the first three command lines listed above can be specified in the command block.
The particular command line selected depends on the mesh-entity type of the variable being ini-
tialized. For example, variables associated with nodes would be initialized if you are using the
NODE SET SUBROUTINE command line, variables associated with faces if you are using the
SURFACE SUBROUTINE command line, and variables associated with elements if you are using
the ELEMENT BLOCK SUBROUTINE command line. The string subroutine_name is the name
of a FORTRAN subroutine that is written by the user.

Following the selected subroutine command line are other command lines that may be used to
implement the user subroutine option. These command lines are described in Section 9.2.2 and
consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL
PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Ex-
amples of using these command lines are provided throughout Chapter 9.

The application of user subroutines for variable initialization is essentially the same as the ap-
application of user subroutines in general. See Section 6.3.7 and Chapter 9 for more details on
implementing the user subroutine option.

When the user subroutine option is used for variable initialization, the user subroutine is called only
once. Also, when a user subroutine is being used, the returned value is the new (initial) variable
value at each mesh entity, and the flags array is ignored.

6.2.6 Additional Command

This command line provides an additional option for the INITIAL CONDITION command block:

   SCALE FACTOR = <real>scale\string (1.0)
Any initial value can be scaled by use of the SCALE FACTOR command line. An initial value generated by any one of the three initial-value-setting options in this command block (i.e., constant magnitude, input mesh, or user subroutine) will be scaled by the real value \texttt{scale_factor}. 
6.3 Kinematic Boundary Conditions

The various kinematic boundary conditions available in Presto are described in this section. The kinematic boundary conditions are nested inside the region scope.

6.3.1 Fixed Displacement Components

BEGIN FIXED DISPLACEMENT
  # {node set commands}
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # specification commands
  COMPONENT = <string>X/Y/Z | COMPONENTS = <string>X/Y/Z
  #
  # additional command
  ACTIVE PERIODS = <string list>period_names
END [FIXED DISPLACEMENT]

The FIXED DISPLACEMENT command block fixes displacement components (X, Y, Z, or some combination thereof) for a set of nodes. This command block contains two groups of commands—node set and component. Each of these command groups is basically independent of the other. In addition to the command lines in the two command groups, there is an additional command line: ACTIVE PERIODS. The ACTIVE PERIODS command line is used to activate or deactivate this kinematic boundary condition for certain time periods. Following are descriptions of the different command groups and the ACTIVE PERIODS command line.

6.3.1.1 Node Set Commands

The {node set commands} portion of the FIXED DISPLACEMENT command block specifies the nodes associated with the boundary condition. This portion of the command block can include some combination of the following command lines:

  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one NODE SET, SURFACE, BLOCK, or INCLUDE ALL BLOCKS command line in the command block.

6.3.1.2 Specification Commands

There are two component specification commands available in the FIXED DISPLACEMENT command block:

\[ \text{COMPONENT} = X/Y/Z \mid \text{COMPONENTS} = X/Y/Z \]

The displacement components that are to be fixed can be specified with either the COMPONENT command line or the COMPONENTS command line. There can be only one COMPONENT command line or one COMPONENTS command line in the command block. The user can specify any combination of the components to be fixed, as in X, Z, X Z, Y X, etc.

6.3.1.3 Additional Command

The ACTIVE PERIODS command line can optionally appear in the FIXED DISPLACEMENT command block:

\[ \text{ACTIVE PERIODS} = \langle \text{string list}\rangle \text{period_names} \]

This command line determines when the boundary condition is active. See Section 2.5 for more information about this optional command line.
6.3.2 Prescribed Displacement

BEGIN PRESERVED DISPLACEMENT
  # {node set commands}
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # specification commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z |
    CYLINDRICAL AXIS = <string>defined_axis |
    RADIAL AXIS = <string>defined_axis
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
END [PRESCRIBED DISPLACEMENT]

The PRESCRIBED DISPLACEMENT command block prescribes a displacement field for a given set of nodes. The displacement field associates a vector giving the magnitude and direction of the displacement with each node in the node set. The displacement field may vary over time and space. If the displacement field has only a time-varying magnitude and uses one of four methods for setting direction, the specification commands in the above command block can be used to specify the displacement field. If the displacement field is more complex, a user subroutine is used to specify the displacement field. You cannot use both the specification commands and the user subroutine commands in the same command block.

The PRESCRIBED DISPLACEMENT command block contains three groups of commands—node set, function, and user subroutine. Each of these command groups is basically independent of the others. In addition to the command lines in the three command groups, there are two additional command lines: SCALE FACTOR and ACTIVE PERIODS. The SCALE FACTOR command line can
be used in conjunction with either the specification commands or the user subroutine commands. The \texttt{ACTIVE PERIODS} command line is used to activate or deactivate this kinematic boundary condition for certain time periods. Following are descriptions of the different command groups and the \texttt{SCALE FACTOR} and \texttt{ACTIVE PERIODS} command lines.

\subsection*{6.3.2.1 Node Set Commands}

The \{node set commands\} portion of the \texttt{PRESCRIBED DISPLACEMENT} command block defines a set of nodes associated with the prescribed displacement field and can include some combination of the following command lines:

\begin{verbatim}
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
\end{verbatim}

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one \texttt{NODE SET}, \texttt{SURFACE}, \texttt{BLOCK}, or \texttt{INCLUDE ALL BLOCKS} command line in the command block.

\subsection*{6.3.2.2 Specification Commands}

If the specification commands are used, the displacement vector at any given time is the same for all nodes in the node set associated with the particular \texttt{PRESCRIBED DISPLACEMENT} command block.

Following are the command lines used to specify the prescribed displacement with a direction and a function:

\begin{verbatim}
DIRECTION = <string>defined_direction |
COMPONENT = <string>X|Y|Z |
CYLINDRICAL AXIS = <string>defined_axis |
RADIAL AXIS = <string>defined_axis
FUNCTION = <string>function_name
\end{verbatim}

The displacement can be specified along an arbitrary user-defined direction, along a component direction (X, Y, or Z), along the azimuthal direction in a cylindrical coordinate system (defined in reference to an axis), or along a radial direction (defined in reference to an axis). Only one of these options (i.e., command lines) is allowed. The displacement is prescribed only in the specified direction. A prescribed displacement boundary condition does not influence the motion in directions orthogonal to the prescribed direction.
- The **DIRECTION** command line is used to prescribe displacement in an arbitrary user-defined direction. The name in the string `defined_direction` is a reference to a direction, which is defined using the **DEFINE DIRECTION** command block within the domain scope.

- The **COMPONENT** command line is used to specify that the prescribed displacement vector lies along one of the component directions. The **COMPONENT** command line is a shortcut to an internally defined direction vector; for example, component \( x \) corresponds to using direction vector \((1, 0, 0)\).

- The **CYLINDRICAL AXIS** command line is used to specify that the prescribed displacement is to be applied in the azimuthal direction of a cylindrical coordinate system. The string `defined_axis` refers to the name of the axis of the cylindrical coordinate system, and which is defined via a **DEFINE AXIS** command block in the domain scope. The displacement is prescribed as a rotation in radians about the axis. Nodes with this type of boundary condition are free to move in the radial and height directions in the cylindrical coordinate system. Restraints can be placed on the nodeset in those directions if desired by applying separate kinematic boundary conditions that contain **RADIAL AXIS** or **DIRECTION** commands that refer to the same axis. Note that this type of boundary condition is not a rotational boundary condition; it only affects translational degrees of freedom.

- The **RADIAL AXIS** command line requires an axis definition that appears in the domain scope. The string `defined_axis` uses an `axis_name` that is defined in the domain scope (via a **DEFINE AXIS** command line). For this option, a radial line is drawn from a node to the radial axis. The prescribed displacement vector lies along this radial line from the node to the radial axis.

The magnitude of the displacement is specified by the **FUNCTION** command line. This references a `function_name` (defined in the domain scope using a **DEFINITION FOR FUNCTION** command block) that specifies the magnitude of the displacement vector as a function of time. The magnitude can be scaled by use of the **SCALE FACTOR** command line described in Section 6.3.2.4.

### 6.3.2.3 User Subroutine Commands

If the user subroutine option is used, the displacement vector may vary spatially at any given time for each of the nodes in the node set associated with the particular **PRESCRIBED DISPLACEMENT** command block. The user subroutine option allows for a more complex description of the displacement field than do the specification commands, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a displacement direction and a magnitude for every node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the displacement field.

Following are the command lines related to the user subroutine option:

```plaintext
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
```
SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value

The user subroutine option is invoked by using the **NODE SET SUBROUTINE** command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user.

Following the **NODE SET SUBROUTINE** command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 9.2.2 and consist of **SUBROUTINE DEBUGGING OFF**, **SUBROUTINE DEBUGGING ON**, **SUBROUTINE REAL PARAMETER**, **SUBROUTINE INTEGER PARAMETER**, and **SUBROUTINE STRING PARAMETER**. Examples of using these command lines are provided throughout Chapter 9.

The magnitude set in the user subroutine can be scaled by use of the **SCALE FACTOR** command line, as described in Section 6.3.2.4.

See Section 6.3.7 and Chapter 9 for more details on implementing the user subroutine option.

### 6.3.2.4 Additional Commands

These command lines in the **PRESCRIBED DISPLACEMENT** command block provide additional options for the boundary condition:

- **SCALE FACTOR** = <real>scale_factor(1.0)
- **ACTIVE PERIODS** = <string list>period_names

The **SCALE FACTOR** command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the displacement in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the displacement from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The **ACTIVE PERIODS** command line determines when the boundary condition is active. See Section 2.5 for more information about this command line.
CHAPTER 6. BOUNDARY CONDITIONS AND INITIAL CONDITIONS

6.3.3 Prescribed Velocity

BEGIN PRESCRIBED VELOCITY
# {node set commands}
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
#
# specification commands
DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z |
    CYLINDRICAL AXIS = <string>defined_axis |
    RADIAL AXIS = <string>defined_axis
FUNCTION = <string>function_name
#
# user subroutine commands
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
#
# additional commands
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
END [PRESCRIBED VELOCITY]

The PRESCRIBED VELOCITY command block prescribes a velocity field for a given set of nodes. The velocity field associates a vector giving the magnitude and direction of the velocity with each node in the node set. The velocity field may vary over time and space. If the velocity field has only a time-varying magnitude and uses one of four methods for setting direction, the specification commands in the above command block can be used to specify the velocity field. If the velocity field is more complex, a user subroutine is used to specify the velocity field. You cannot use both the specification commands and the user subroutine commands in the same command block.

The PRESCRIBED VELOCITY command block contains three groups of commands—node set, function, and user subroutine. Each of these command groups is basically independent of the others. In addition to the command lines in the three command groups, there are two additional command lines: SCALE FACTOR and ACTIVE PERIODS. The SCALE FACTOR command line can be used in conjunction with either the specification commands or the user subroutine commands.
6.3. KINEMATIC BOUNDARY CONDITIONS

The **ACTIVE PERIODS** command line is used to activate or deactivate this kinematic boundary condition for certain time periods. Following are descriptions of the different command groups and the **SCALE FACTOR** and **ACTIVE PERIODS** command lines.

### 6.3.3.1 Node Set Commands

The `{node set commands}` portion of the **PRESCRIBED VELOCITY** command block defines a set of nodes associated with the prescribed velocity field and can include some combination of the following command lines:

- **NODE SET** = `<string list>`nodelist_names
- **SURFACE** = `<string list>`surface_names
- **BLOCK** = `<string list>`block_names
- **INCLUDE ALL BLOCKS**
- **REMOVE NODE SET** = `<string list>`nodelist_names
- **REMOVE SURFACE** = `<string list>`surface_names
- **REMOVE BLOCK** = `<string list>`block_names

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one **NODE SET**, **SURFACE**, **BLOCK**, or **INCLUDE ALL BLOCKS** command line in the command block.

### 6.3.3.2 Specification Commands

If the specification commands are used, the velocity vector at any given time is the same for all nodes in the node set associated with the particular **PRESCRIBED VELOCITY** command block.

Following are the command lines used to specify the prescribed velocity with a direction and a function:

- **DIRECTION** = `<string>defined_direction`  |
- **COMPONENT** = `<string>X|Y|Z`  |
- **CYLINDRICAL AXIS** = `<string>defined_axis`  |
- **RADIAL AXIS** = `<string>defined_axis`  |
- **FUNCTION** = `<string>function_name`  |

The velocity can be specified along an arbitrary user-defined direction, along a component direction (X, Y, or Z), along the azimuthal direction in a cylindrical coordinate system (defined in reference to an axis), or along a radial direction (defined in reference to an axis). Only one of these options (i.e., command lines) is allowed. The velocity is prescribed only in the specified direction. A prescribed velocity boundary condition does not influence the motion in directions orthogonal to the prescribed direction.

- **The DIRECTION command line** is used to prescribe velocity in an arbitrary user-defined direction. The name in the string **defined_direction** is a reference to a direction, which is defined using the **DEFINE DIRECTION** command block within the domain scope.
- The `COMPONENT` command line is used to specify that the prescribed velocity vector lies along one of the component directions. The `COMPONENT` command line is a shortcut to an internally defined direction vector; for example, `component x` corresponds to using direction vector \((1, 0, 0)\).

- The `CYLINDRICAL AXIS` command line is used to specify that the prescribed velocity is to be applied in the azimuthal direction of a cylindrical coordinate system. The string `defined_axis` refers to the name of the axis of the cylindrical coordinate system, and which is defined via a `DEFINE AXIS` command block in the domain scope. The velocity is prescribed as a rotation in radians about the axis. Nodes with this type of boundary condition are free to move in the radial and height directions in the cylindrical coordinate system. Restraints can be placed on the nodeset in those directions if desired by applying separate kinematic boundary conditions that contain `RADIAL AXIS` or `DIRECTION` commands that refer to the same axis. Note that this type of boundary condition is not a rotational boundary condition; it only affects translational degrees of freedom.

- The `RADIAL AXIS` command line requires an axis definition that appears in the domain scope. The string `defined_axis` uses an `axis_name` that is defined in the domain scope (via a `DEFINE AXIS` command line). For this option, a radial line is drawn from a node to the radial axis. The velocity vector lies along this radial line from the node to the radial axis. The magnitude of the velocity is specified by the `FUNCTION` command line. This references a `function_name` (defined in the domain scope using a `DEFINITION FOR FUNCTION` command block) that specifies the magnitude of the velocity vector as a function of time. The magnitude can be scaled by use of the `SCALE FACTOR` command line described in Section 6.3.3.4.

### 6.3.3.3 User Subroutine Commands

If the user subroutine option is used, the velocity vector may vary spatially at any given time for each of the nodes in the node set associated with the particular `PRESCRIBED VELOCITY` command block. The user subroutine option allows for a more complex description of the velocity field than do the specification commands, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a velocity direction and a magnitude for every node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the velocity field.

Following are the command lines related to the user subroutine option:

```
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
                   = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
                   = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
                   = <string>param_value
```
The user subroutine option is invoked by using the **NODE SET SUBROUTINE** command line. The string `subroutine_name` is the name of a FORTRAN subroutine that is written by the user.

Following the **NODE SET SUBROUTINE** command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 9.2.2 and consist of **SUBROUTINE DEBUGGING OFF**, **SUBROUTINE DEBUGGING ON**, **SUBROUTINE REAL PARAMETER**, **SUBROUTINE INTEGER PARAMETER**, and **SUBROUTINE STRING PARAMETER**. Examples of using these command lines are provided throughout Chapter 9.

The magnitude set in the user subroutine can be scaled by use of the **SCALE FACTOR** command line, as described in Section 6.3.3.4.

### 6.3.3.4 Additional Commands

These command lines in the **PRESCRIBED VELOCITY** command block provide additional options for the boundary condition:

- **SCALE FACTOR** = `<real>scale_factor(1.0)`
- **ACTIVE PERIODS** = `<string list>period_names`

The **SCALE FACTOR** command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the velocity in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the velocity from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The **ACTIVE PERIODS** command line determines when the boundary condition is active. See Section 2.5 for more information about this command line.
6.3.4 Prescribed Acceleration

BEGIN PRESCRIBED ACCELERATION
  # {node set commands}
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # specification commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
END [PRESCRIBED ACCELERATION]

The PRESCRIBED ACCELERATION command block prescribes an acceleration field for a given set of nodes. The acceleration field associates a vector giving the magnitude and direction of the acceleration with each node in the node set. The acceleration field may vary over time and space. If the acceleration field has only a time-varying component, the specification commands in the above command block can be used to specify the acceleration field. If the acceleration field has both time-varying and spatially varying components, a user subroutine is used to specify the acceleration field. You cannot use both the specification commands and the user subroutine commands in the same command block.

The PRESCRIBED ACCELERATION command block contains three groups of commands—node set, function, and user subroutine. Each of these command groups is basically independent of the others. In addition to the command lines in the three command groups, there are two additional command lines: SCALE FACTOR and ACTIVE PERIODS. The SCALE FACTOR command line can be used in conjunction with either the specification commands or the user subroutine commands. The ACTIVE PERIODS command line is used to activate or deactivate this kinematic boundary.
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Condition for certain time periods. Following are descriptions of the different command groups and the **SCALE FACTOR** and **ACTIVE PERIODS** command lines.

### 6.3.4.1 Node Set Commands

The `{node set commands}` portion of the PRESCRIBED ACCELERATION command block defines a set of nodes associated with the prescribed acceleration field and can include some combination of the following command lines:

- **NODE SET** = `<string list>nodelist_names`
- **SURFACE** = `<string list>surface_names`
- **BLOCK** = `<string list>block_names`
- **INCLUDE ALL BLOCKS**
- **REMOVE NODE SET** = `<string list>nodelist_names`
- **REMOVE SURFACE** = `<string list>surface_names`
- **REMOVE BLOCK** = `<string list>block_names`

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one NODE SET, SURFACE, BLOCK, or INCLUDE ALL BLOCKS command line in the command block.

### 6.3.4.2 Specification Commands

If the specification commands are used, the acceleration vector at any given time is the same for all nodes in the node set associated with the particular PRESCRIBED ACCELERATION command block. The direction of the acceleration vector is constant for all time; the magnitude of the acceleration vector may vary with time, however.

Following are the command lines used to specify the prescribed acceleration with a direction and a function:

- **DIRECTION** = `<string>defined_direction`
- **COMPONENT** = `<string>X|Y|Z`
- **FUNCTION** = `<string>function_name`

The acceleration can be specified either along an arbitrary user-defined direction or along a component direction (X, Y, or Z), but not both. The acceleration is prescribed only in the specified direction. A prescribed acceleration boundary condition does not influence the motion in directions orthogonal to the prescribed direction.

- The **DIRECTION** command line is used to prescribe acceleration in an arbitrary user-defined direction. The name in the string `defined_direction` is a reference to a direction, which is defined using the **DEFINE DIRECTION** command block within the domain scope.
- The COMPONENT command line is used to specify that the prescribed acceleration vector lies along one of the component directions. The COMPONENT command line is a shortcut to an internally defined direction vector; for example, component $x$ corresponds to using direction vector $(1, 0, 0)$.

The magnitude of the acceleration is specified by the FUNCTION command line. This references a function_name (defined in the domain scope using a DEFINITION FOR FUNCTION command block) that specifies the magnitude of the acceleration vector as a function of time. The magnitude can be scaled by use of the SCALE FACTOR command line described in Section 6.3.4.4.

### 6.3.4.3 User Subroutine Commands

If the user subroutine option is used, the acceleration vector may vary spatially at any given time for each of the nodes in the node set associated with the particular PRESCRIBED ACCELERATION command block. The user subroutine option allows for a more complex description of the acceleration field than do the specification commands, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define an acceleration direction and a magnitude for every node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the acceleration field.

Following are the command lines related to the user subroutine option:

```
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name = <string>param_value
```

The user subroutine option is invoked by using the NODE SET SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user.

Following the NODE SET SUBROUTINE command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 9.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided throughout Chapter 9.

The magnitude set in the user subroutine can be scaled by use of the SCALE FACTOR command line, as described in Section 6.3.4.4.

See Section 6.3.7 and Chapter 9 for more details on implementing the user subroutine option.
6.3.4.4 Additional Commands

These command lines in the PRESCRIBED ACCELERATION command block provide additional options for the boundary condition:

\[
\begin{align*}
\text{SCALE FACTOR} & = <\text{real}> \text{scale\_factor}(1.0) \\
\text{ACTIVE PERIODS} & = <\text{string list}> \text{period\_names}
\end{align*}
\]

The SCALE FACTOR command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the acceleration in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the acceleration from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The ACTIVE PERIODS command line determines when the boundary condition is active. See Section 2.5 for more information about this command line.
6.3.5 Fixed Rotation

BEGIN FIXED ROTATION
  # {node set commands}
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # specification commands
  COMPONENT = <string>X/Y/Z | COMPONENTS = <string>X/Y/Z
  #
  # additional command
  ACTIVE PERIODS = <string list>periods_names
END [FIXED ROTATION]

The **FIXED ROTATION** command block fixes rotation about direction components (X, Y, Z, or some combination thereof) for a set of nodes. This command block contains two groups of commands—node set and component. Each of these command groups is basically independent of the other. In addition to the command lines in the two command groups, there is an additional command line: **ACTIVE PERIODS**. The **ACTIVE PERIODS** command line is used to activate or deactivate this kinematic boundary condition for certain time periods. Following are descriptions of the different command groups and the **ACTIVE PERIODS** command line.

6.3.5.1 Node Set Commands

The **{node set commands}** portion of the command block specifies the nodes associated with the boundary condition. This portion of the command block can include some combination of the following command lines:

- **NODE SET = <string list>nodelist_names**
- **SURFACE = <string list>surface_names**
- **BLOCK = <string list>block_names**
- **INCLUDE ALL BLOCKS**
- **REMOVE NODE SET = <string list>nodelist_names**
- **REMOVE SURFACE = <string list>surface_names**
- **REMOVE BLOCK = <string list>block_names**

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one **NODE SET, SURFACE, BLOCK, or INCLUDE ALL BLOCKS** command line in the command block.
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6.3.5.2 **Specification Commands**

There are two component specification commands available in the `FIXED ROTATION` command block:

\[
\text{COMPONENT} = X/Y/Z \mid \text{COMPONENTS} = X/Y/Z
\]

The rotation components that are to be fixed can be specified with either the `COMPONENT` command line or the `COMPONENTS` command line. There can be only one `COMPONENT` command line or one `COMPONENTS` command line in the command block. The user can specify any combination of the components to be fixed, as in \(X, Z, X\), \(Z, Y\), \(X\), etc.

6.3.5.3 **Additional Command**

The `ACTIVE PERIODS` command line can optionally appear in the `FIXED ROTATION` command block:

\[
\text{ACTIVE PERIODS} = <\text{string list}> \text{period_names}
\]

This command line determines when the boundary condition is active. See Section 2.5 for more information about this optional command line.
6.3.6 Prescribed Rotation

BEGIN PRESCRIBED ROTATION
  # {node set commands}
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # specification commands
  DIRECTION = <string>defined_direction |
             COMPONENT = <string>X|Y|Z
  FUNCTION = <string>function_name
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
     = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
     = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
     = <string>param_value
  #
  # additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
END [PRESCRIBED ROTATION]

The PRESCRIBED ROTATION command block prescribes the rotation about an axis for a given set of nodes. The rotation field associates a vector giving the magnitude and direction of the rotation with each node in the node set. The rotation field may vary over time and space. If the rotation field has only a time-varying component, the specification commands in the above command block can be used to specify the rotation field. If the rotation field has both time-varying and spatially varying components, a user subroutine is used to specify the rotation field. You cannot use both the specification commands and the user subroutine commands in the same command block.

The PRESCRIBED ROTATION command block contains three groups of commands—node set, function, and user subroutine. Each of these command groups is basically independent of the others. In addition to the command lines in the three command groups, there are two additional command lines: SCALE FACTOR and ACTIVE PERIODS. The SCALE FACTOR command line can be used in conjunction with either the specification commands or the user subroutine commands. The ACTIVE PERIODS command line is used to activate or deactivate this kinematic boundary condition for certain time periods. Following are descriptions of the different command groups.
and the \texttt{SCALE FACTOR} and \texttt{ACTIVE PERIODS} command lines.

### 6.3.6.1 Node Set Commands

The \texttt{NODE SET Commands} portion of the \texttt{PRESCRIBED ROTATION} command block defines a set of nodes associated with the prescribed rotation field and can include some combination of the following command lines:

- \texttt{NODE SET} = \texttt{<string list>nodelist_names}
- \texttt{SURFACE} = \texttt{<string list>surface_names}
- \texttt{BLOCK} = \texttt{<string list>block_names}
- \texttt{INCLUDE ALL BLOCKS}
- \texttt{REMOVE NODE SET} = \texttt{<string list>nodelist_names}
- \texttt{REMOVE SURFACE} = \texttt{<string list>surface_names}
- \texttt{REMOVE BLOCK} = \texttt{<string list>block_names}

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one \texttt{NODE SET}, \texttt{SURFACE}, \texttt{BLOCK}, or \texttt{INCLUDE ALL BLOCKS} command line in the command block.

### 6.3.6.2 Specification Commands

If the specification commands are used, the rotation vector at any given time is the same for all nodes in the node set associated with the particular \texttt{PRESCRIBED ROTATION} command block. The direction of the rotation vector is constant for all time; the magnitude of the rotation vector may vary with time, however.

Following are the command lines used to specify the prescribed rotation with a direction and a function:

- \texttt{DIRECTION} = \texttt{<string>defined_direction |}
- \texttt{COMPONENT} = \texttt{<string>X|Y|Z}
- \texttt{FUNCTION} = \texttt{<string>function_name}

The rotation can be specified either along an arbitrary user-defined direction or along a component direction (X, Y, or Z), but not both. The rotation is prescribed only in the specified direction. A prescribed rotation boundary condition does not influence the rotation in directions orthogonal to the prescribed direction.

- The \texttt{DIRECTION} command line is used to prescribe rotation in an arbitrary user-defined direction. The name in the string \texttt{defined_direction} is a reference to a direction, which is defined using the \texttt{DEFINE DIRECTION} command block within the domain scope.

- The \texttt{COMPONENT} command line is used to specify that the prescribed rotation vector lies along one of the component directions. The \texttt{COMPONENT} command line is a shortcut to an
internally defined direction vector; for example, component x corresponds to using direction vector (1, 0, 0).

The magnitude of the rotation is specified by the FUNCTION command line. This references a function_name (defined in the domain scope in a DEFINITION FOR FUNCTION command block) that specifies the magnitude of the rotation vector as a function of time. The magnitude can be scaled by use of the SCALE FACTOR command line described in Section 6.3.6.4.

The magnitude of the rotation, as specified by the product of the function and the scale factor, has units of radians per second.

6.3.6.3 User Subroutine Commands

If the user subroutine option is used, the rotation vector may vary spatially at any given time for each of the nodes in the node set associated with the particular PRESCRIBED ROTATION command block. The user subroutine option allows for a more complex description of the rotation field than do the specification commands, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a rotation direction and a magnitude for every node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the rotation field.

Following are the command lines related to the user subroutine option:

- NODE SET SUBROUTINE = <string>subroutine_name
- SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
- SUBROUTINE REAL PARAMETER: <string>param_name = <real>param_value
- SUBROUTINE INTEGER PARAMETER: <string>param_name = <integer>param_value
- SUBROUTINE STRING PARAMETER: <string>param_name = <string>param_value

The user subroutine option is invoked by using the NODE SET SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user.

Following the NODE SET SUBROUTINE command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 9.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided throughout Chapter 9.

The magnitude set in the user subroutine can be scaled by use of the SCALE FACTOR command line, as described in Section 6.3.6.4.

See Section 6.3.7 and Chapter 9 for more details on implementing the user subroutine option.
6.3.6.4 Additional Commands

These command lines in the PRESCRIBED ROTATION command block provide additional options for the boundary condition:

```
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
```

The SCALE FACTOR command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the rotation in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the rotation from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The ACTIVE PERIODS command line determines when the boundary condition is active. See Section 2.5 for more information about this command line.
6.3.7 Subroutine Usage for Kinematic Boundary Conditions

The prescribed kinematic boundary conditions may be defined by a user subroutine. All these conditions use a node set subroutine. See Chapter 9 for an in-depth discussion of user subroutines. The kinematic boundary conditions will be applied to nodes. The subroutine that you write will have to return six output values per node and one output flag per node. The usage of the output values depends on the returned flag value for a node, as follows:

- If the flag value is negative, no constraint will be applied to the node.
- If the flag value is equal to zero, the constraint will be absolute. All components of the boundary condition will be specified. For example, suppose you have written a user subroutine to be called from a prescribed displacement subroutine. The prescribed displacements are to be passed through an array `output_values`. For a given node `inode`, the `output_values` array would have the following values:

  - `output_values(1,inode)` = displacement in x at inode
  - `output_values(2,inode)` = displacement in y at inode
  - `output_values(3,inode)` = displacement in z at inode
  - `output_values(4,inode)` = not used
  - `output_values(5,inode)` = not used
  - `output_values(6,inode)` = not used

- If the flag value is equal to one, the constraint will be a specified amount in a given direction. For example, suppose you have written a user subroutine to be called from a prescribed displacement subroutine. The prescribed displacements are to be passed through an array `output_values`. For a given node `inode`, the `output_values` array would have the following values:

  - `output_values(1,inode)` = magnitude of displacement
  - `output_values(2,inode)` = not used
  - `output_values(3,inode)` = not used
  - `output_values(4,inode)` = x component of direction vector
  - `output_values(5,inode)` = y component of direction vector
  - `output_values(6,inode)` = z component of direction vector

The direction in which the constraint will act is given by `output_values 4 through 6 for inode`. The magnitude of the displacement in the specified direction is given by `output_values 1 at inode`. To compute the constraint, Presto first normalizes the direction vector. Next, Presto multiplies the normalized direction vector by the magnitude of the displacement and applies the resultant constraint vector.

Displacements or velocities orthogonal to the prescribed direction will not be constrained. (This is true regardless of whether or not one uses a user subroutine for the prescribed kinematic boundary conditions.) Take the case of a prescribed displacement condition. The displacement orthogonal to a prescribed direction of motion depends on the internal and external forces orthogonal to the prescribed direction. Displacement orthogonal to the prescribed direction may or may not be zero.
6.4 Initial Velocity Conditions

BEGIN INITIAL VELOCITY
  # {node set commands}
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # direction specification commands
  COMPONENT = <string>X|Y|Z |
  DIRECTION = <string>defined_direction
  MAGNITUDE = <real>magnitude_of_velocity
  #
  # angular velocity specification commands
  CYLINDRICAL AXIS = <string>defined_axis
  ANGULAR VELOCITY = <real>angular_velocity
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
      = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
      = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
      = <string>param_value
END [INITIAL VELOCITY]

The INITIAL VELOCITY command block specifies an initial velocity field for a set of nodes. There are two simple options for specifying the initial velocity field: by direction and by angular velocity. The user subroutine option available is also available to specify an initial velocity. You may use only one of the available options—direction specification, angular velocity specification, or user subroutine.

The INITIAL VELOCITY command block contains four groups of commands—node set, direction specification, angular velocity specification, and user subroutine. Command lines associated with the node set commands must appear. As mentioned, command lines associated with one of the options must also appear. Following are descriptions of the different command groups.
6.4.1 Node Set Commands

The {node set commands} portion of the INITIAL VELOCITY command block defines a set of nodes associated with the initial velocity field and can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one NODE SET, SURFACE, BLOCK, or INCLUDE ALL BLOCKS command line in the command block.

6.4.2 Direction Specification Commands

If the direction specification commands are used, the initial velocity is applied along a defined direction with a specific magnitude. Following are the command lines for the direction option:

```
COMPONENT = <string>X|Y|Z |
DIRECTION = <string>defined_direction
MAGNITUDE = <real>magnitude_of_velocity
```

The initial velocity can be specified either along an arbitrary user-defined direction or along a component direction (X, Y, or Z), but not both. The velocity is prescribed only in the specified direction. A prescribed velocity boundary condition does not influence the movement in directions orthogonal to the prescribed direction.

- The DIRECTION command line is used to prescribe initial velocity in an arbitrary user-defined direction. The name in the string defined_direction is a reference to a direction, which is defined using the DEFINE DIRECTION command block within the domain scope.

- The COMPONENT command line is used to specify that the initial velocity vector lies along one of the component directions. The COMPONENT command line is a shortcut to an internally defined direction vector; for example, component x corresponds to using direction vector (1, 0, 0).

The magnitude of the initial velocity is given by the MAGNITUDE command line with the real value magnitude_of_velocity.

Either the COMPONENT command line or the DIRECTION command line must be specified with the MAGNITUDE command line if you use the direction specification commands.
6.4.3 Angular Velocity Specification Commands

If the angular velocity specification commands are used, the initial velocity is applied as an initial angular velocity about some axis. Following are the command lines for angular velocity specification:

\[
\text{CYLINDRICAL AXIS} = \text{<string>defined_axis }
\text{ANGULAR VELOCITY} = \text{<real>angular_velocity}
\]

The axis about which the body is initially rotating is given by the CYLINDRICAL AXIS command line. The string defined_axis uses an axis_name that is defined in the domain scope (via a DEFINE AXIS command line).

The magnitude of the angular velocity about this axis is specified by the ANGULAR VELOCITY command line with the real value angular_velocity. This value is specified in units of radians per unit of time. Typically, the value for the angular velocity will be radians per second.

Both the CYLINDRICAL AXIS command line and the ANGULAR VELOCITY command line are required if you use the angular velocity specification commands.

6.4.4 User Subroutine Commands

If the user subroutine option is used, the initial velocity vector may vary spatially at any given time for each of the nodes in the node set associated with the particular INITIAL CONDITION command block. The user subroutine option allows for a more complex description of the initial velocity field than do the direction and angular-velocity options, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a velocity direction and a magnitude for every node to which the initial velocity field will be applied. The subroutine will be called by Presto at the appropriate time to generate the initial velocity field.

Following are the command lines related to the user subroutine option:

\[
\text{NODE SET SUBROUTINE} = \text{<string>subroutine_name }
\text{SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON}
\text{SUBROUTINE REAL PARAMETER: <string>param_name = <real>param_value}
\text{SUBROUTINE INTEGER PARAMETER: <string>param_name = <integer>param_value}
\text{SUBROUTINE STRING PARAMETER: <string>param_name = <string>param_value}
\]

The user subroutine option is invoked by using the NODE SET SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user.

Following the NODE SET SUBROUTINE command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 9.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL
PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided throughout Chapter 9.

See Section 6.3.7 and Chapter 9 for more details on implementing the user subroutine option.
6.5 Force Boundary Conditions

A variety of force boundary conditions are available in Presto. This section describes these boundary conditions.

6.5.1 Pressure

BEGIN PRESSURE

# {surface set commands}
SURFACE = <string list>surface_names
REMOVE SURFACE = <string list>surface_names
#
# specification command
FUNCTION = <string>function_name
#
# user subroutine commands
SURFACE SUBROUTINE = <string>subroutine_name |
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
#
# external pressure sources
READ VARIABLE = <string>variable_name
OBJECT TYPE = <string>NODE|FACE(NODE)
TIME = <real>time
FIELD VARIABLE = <string>field_variable
#
# output external forces from pressure
EXTERNAL FORCE CONTRIBUTION OUTPUT NAME =
  <string>variable_name
#
# additional commands
USE DEATH = <string>death_name
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
END [PRESSURE]

The PRESSURE command block applies a pressure to each face in the associated surfaces. The pressure field can either be constant over the faces and vary in time, or it can be determined by a user subroutine. If the pressure field is constant over the faces and has only a time-varying component, the function command in the above command block can be used to specify the pressure.
field. If the pressure field has both time-varying and spatially varying components, user subroutine commands are used to specify the pressure field. The pressure field may also be obtained from a mesh file or from another SIERRA code through a transfer operator. You can use only one of these four options—function, user subroutine, mesh file, transfer from another code—to specify the pressure field.

Currently, the **PRESSURE** command block can be used for surfaces that have faces derived from solid elements (eight-node hexahedra, four-node tetrahedra, eight-node tetrahedra, etc.), membranes, and shells.

A pressure boundary condition generates nodal forces that are summed into the external force vector that is used to calculate the motion of a body. The external force vector contains the contribution from all forces acting on the body. There is an option in the **PRESSURE** command block to save information about the contribution to the external force vector due only to pressure loads. This option does not change the magnitude or time history of the pressure load (regardless of how they are defined), but merely stores information in a user-accessible variable.

The **PRESSURE** command block contains five groups of commands—surface set, function, user subroutine, external pressure, and output external forces. Each of these command groups is basically independent of the others. In addition to the command lines in the five command groups, there are three additional command lines: **USE DEATH**, **SCALE FACTOR** and **ACTIVE PERIODS**.

The **USE DEATH** command line links the pressure boundary condition to an element death definition so that the underlying surface geometry is updated as elements are killed. The **SCALE FACTOR** command line can be used in conjunction with either the function command or the user subroutine commands. The **ACTIVE PERIODS** command line is used to activate or deactivate this force boundary condition for certain time periods. Following are descriptions of the different command groups and the **USE DEATH**, **SCALE FACTOR**, and **ACTIVE PERIODS** command lines.

### 6.5.1.1 Surface Set Commands

The {surface set commands} portion of the **PRESSURE** command block defines a set of surfaces associated with the pressure field and can include some combination of the following command lines:

- \texttt{SURFACE = <string list>surface\_names}
- \texttt{REMOVE SURFACE = <string list>surface\_names}

In the **SURFACE** command line, you can list a series of surfaces through the string list \texttt{surface\_names}. There must be at least one **SURFACE** command line in the command block. The **REMOVE SURFACE** command line allows you to delete surfaces from the set specified in the **SURFACE** command line(s) through the string list \texttt{surface\_names}. See Section 6.1.1 for more information about the use of these command lines for creating a set of surfaces used by the boundary condition.

### 6.5.1.2 Specification Commands

If the function command is used, the pressure vector at any given time is the same for all surfaces associated with the particular **PRESSURE** command block. The direction of the pressure vector is
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constant for all time; the magnitude of the pressure vector may vary with time, however.

Following is the command line used to specify the pressure with a function:

\[
\text{FUNCTION} = \text{<string>function\_name}
\]

The pressure is applied in the opposite direction to the outward normals of the faces that define the surfaces. The magnitude of the pressure is specified by the FUNCTION command line. This references a function\_name (defined in the domain scope in a DEFINITION FOR FUNCTION command block) that specifies the magnitude of the pressure vector as a function of time. The magnitude can be scaled by use of the SCALE FACTOR command line described in Section 6.5.1.6.

6.5.1.3 User Subroutine Commands

If the user subroutine option is used, the pressure may vary spatially at any given time for each of the surfaces associated with the particular PRESSURE command block. The user subroutine option allows for a more complex description of the pressure field than does the function command, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a pressure for every face to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the pressure field.

Following are the command lines related to the user subroutine option:

\[
\begin{align*}
\text{SURFACE SUBROUTINE} & = \text{<string>subroutine\_name} | \\
\text{NODE SET SUBROUTINE} & = \text{<string>subroutine\_name} \\
\text{SUBROUTINE DEBUGGING OFF} & | \text{SUBROUTINE DEBUGGING ON} \\
\text{SUBROUTINE REAL PARAMETER:} & \text{<string>param\_name} = \text{<real>param\_value} \\
\text{SUBROUTINE INTEGER PARAMETER:} & \text{<string>param\_name} = \text{<integer>param\_value} \\
\text{SUBROUTINE STRING PARAMETER:} & \text{<string>param\_name} = \text{<string>param\_value}
\end{align*}
\]

The user subroutine option is invoked by using the SURFACE SUBROUTINE command line or the NODE SET subroutine command line. The string subroutine\_name in both command lines is the name of a FORTRAN subroutine that is written by the user. The particular command line selected depends on the mesh-entity type for which the pressure field is being calculated. Associating pressure values with faces would require the use of a SURFACE SUBROUTINE command line. Associating pressure values with nodes would require the use of a NODE SET SUBROUTINE command line.

Following the selected subroutine command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 9.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided throughout Chapter 9.
The magnitude set in the user subroutine can be scaled by use of the SCALE FACTOR command line, as described in Section 6.5.1.6.

Usage requirements. Following are the usage requirements for the two types of subroutines:

- The surface subroutine operates on a group of faces. The subroutine that you write will return one output value per face. Suppose you write a user subroutine that returns the pressure information through an array output_value. The value output_value(1,iface) corresponds to the average pressure on face iface. The values of the ags array are not used.

- The node set subroutine that you write will return one value per node. Suppose you write a user subroutine that returns the pressure information through an array output_value. The return value output_value(1,inode) is the pressure at the node inode. The total pressure on the each face is found by integrating the pressures at the nodes. The values of the flags array are not used.

See Chapter 9 for more details on implementing the user subroutine option.

6.5.1.4 External Pressure Sources

Pressure may be obtained from two different external sources. The first option for obtaining pressure from an external source uses a mesh file. The commands for obtaining pressure information from a mesh file are as follows:

```
READ VARIABLE = <string>variable_name
OBJECT TYPE = <string>NODE|FACE(NODE)
TIME = <real>time
```

The READ VARIABLE command line specifies the name of the variable on the mesh file, variable_name, that is used to prescribe the pressure field. The OBJECT TYPE command line specifies whether the pressure field on the mesh file is specified for nodes (the mesh object type is NODE) or for faces (the mesh object type is FACE). If the OBJECT TYPE command line is not present, it is assumed that the variable is for nodes. If the TIME command line is present, only the pressure field information at a given time, as set by the time parameter, is read from the mesh file. If the TIME command line is not present, the pressure field information for all times is read. Pressure field information will then be interpolated as necessary during an analysis.

The second option for obtaining pressure from and external sources relies on the transfer of information from another SIERRA code. The command for obtaining pressure information by transfer from another code is:

```
FIELD VARIABLE = <string>variable_name
```

Here variable_name is the name of the registered variable where pressure information is to be stored. The pressure information will be transferred into this registered variable from another SIERRA code via a transfer operator.
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6.5.1.5 Output Command

This command line lets the user create a variable that stores information about the contribution to the external force vector at a node arising solely from a pressure:

```
EXTERNAL FORCE CONTRIBUTION OUTPUT NAME =
<string>variable_name
```

If the above command line appears in a PRESSURE command block, then there will be a variable created with whatever name the user specifies for `variable_name`. The variable defines a three-dimensional vector at each node associated with this particular command block. The three-dimensional vector at each node represents the external force due solely to the pressure on the elements attached to that node. For example, if one of the nodes associated with this particular command block has four elements attached to it and each element has a pressure load, then the external force contribution at the node would be summed from the pressure load for all four elements.

Once this variable for the external force contribution from a pressure load is specified, it may be used like any other registered nodal variable. The user can, for example, specify the variable as a nodal variable to be output in a RESULTS OUTPUT command block. Or the user can reference the variable in a user subroutine.

6.5.1.6 Additional Commands

These command lines in the PRESSURE command block provide additional options for the boundary condition:

```
USE DEATH = <string>death_name
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
```

The `USE DEATH` command line links the pressure boundary condition to an element death definition. The string `death_name` must match a name used in an ELEMENT DEATH command block. When elements are killed by the named element death definition, the pressure boundary condition will be applied to the newly exposed faces.

The `SCALE FACTOR` command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the function command or the user subroutine. For example, if the magnitude of the pressure in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the pressure from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The `ACTIVE PERIODS` command line determines when the boundary condition is active. See Section 2.5 for more information about this command line.
6.5.2 Traction

BEGIN TRACTION
   # {surface set commands}
   SURFACE = <string list>surface_names
   REMOVE SURFACE = <string list>surface_names
   #
   # specification commands
   DIRECTION = <string>direction_name
   FUNCTION = <string>function_name
   #
   # user subroutine commands
   NODE SET SUBROUTINE = <string>subroutine_name
   SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
   SUBROUTINE REAL PARAMETER: <string>param_name
      = <real>param_value
   SUBROUTINE INTEGER PARAMETER: <string>param_name
      = <integer>param_value
   SUBROUTINE STRING PARAMETER: <string>param_name
      = <string>param_value
   #
   # additional commands
   SCALE FACTOR = <real>scale_factor(1.0)
   ACTIVE PERIODS = <string list>period_names
   #
END [TRACTION]

The TRACTION command block applies a traction to each face in the associated surfaces. The traction has units of force per unit area. (A traction, unlike a pressure, may not necessarily be in the direction of the normal to the face to which it is applied.) The given traction is integrated over the surface area of a face.

The traction field can be determined by a SIERRA function or a user subroutine. If the traction field is constant over the faces and has only a time-varying component, the specification commands in the above command block can be used to specify the traction field. If the traction field has both time-varying and spatially varying components, a user subroutine is used to specify the traction field.

The traction field can only be controlled by one method. Accordingly, a TRACTION command block can only contain one of the options: function or user subroutine.

Currently, the TRACTION command block can be used for surfaces that have faces derived from solid elements (eight-node hexahedra, four-node tetrahedra, eight-node tetrahedra, etc.), membranes, and shells.

The TRACTION command block contains three groups of commands—surface set and user subroutine. Each of these command groups is basically independent of the others. In addition to the command lines in the four command groups, there are two additional command lines: SCALE FACTOR and ACTIVE PERIODS. The SCALE FACTOR command line can be used in conjunction with the
specification commands or the user subroutine option. The active periods command line is used to activate or deactivate this force boundary condition for certain time periods. Following are descriptions of the different command groups and the scale factor and active periods command lines.

### 6.5.2.1 Surface Set Commands

The {surface set commands} portion of the traction command block defines a set of surfaces associated with the traction field and can include some combination of the following command lines:

- **SURFACE** = <string list>surface_names
- **REMOVE SURFACE** = <string list>surface_names

In the SURFACE command line, you can list a series of surfaces through the string list surface_names. There must be at least one SURFACE command line in the command block. The REMOVE SURFACE command line allows you to delete surfaces from the set specified in the SURFACE command line(s) through the string list surface_names. See Section 6.1.1 for more information about the use of these command lines for creating a set of surfaces used by the boundary condition.

### 6.5.2.2 Specification Commands

If the specification commands are used, the traction vector at any given time is the same for all surfaces associated with the particular traction command block. The direction of the traction vector is constant for all time; the magnitude of the traction vector may vary with time, however. Following are the command lines used to specify the traction with a direction and a function:

- **DIRECTION** = <string>defined_direction
- **FUNCTION** = <string>function_name

The traction is specified in an arbitrary user-defined direction, and is defined using the DIRECTION command line. The name in the string defined_direction is a reference to a direction, which is defined using the DEFINE DIRECTION command block within the domain scope.

The magnitude of the traction is specified by the FUNCTION command line. This references a function_name (defined in the domain scope in a DEFINITION FOR FUNCTION command block) that specifies the magnitude of the traction vector as a function of time. The magnitude can be scaled by use of the scale factor command line described in Section 6.5.2.4.

### 6.5.2.3 User Subroutine Commands

If the user subroutine option is used, the traction vector may vary spatially at any given time for each of the surfaces associated with the particular traction command block. The user subroutine option allows for a more complex description of the traction field than does the function option, but the user subroutine option also requires that you write a user subroutine to implement this...
capability. The user subroutine will be used to define a traction for every face to which the bound-
ary condition will be applied. The subroutine will be called by Presto at the appropriate time to
generate the traction field.

Following is the command line related to the user subroutine option:

\[
\text{NODE SET SUBROUTINE = <string>subroutine_name}\]
\[
\text{SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON}\]
\[
\text{SUBROUTINE REAL PARAMETER: <string>param_name} = <real>param_value\]
\[
\text{SUBROUTINE INTEGER PARAMETER: <string>param_name} = <integer>param_value\]
\[
\text{SUBROUTINE STRING PARAMETER: <string>param_name} = <string>param_value\]

The user subroutine option is invoked by using the \text{NODE SET} subroutine command line. The
string \text{subroutine_name} is the name of a FORTRAN subroutine that is written by the user.
Associating traction values with nodes requires the use of a \text{NODE SET SUBROUTINE} command
line.

Following the \text{NODE SET SUBROUTINE} command line are other command lines that may be used
to implement the user subroutine option. These command lines are described in Section 9.2.2 and
consist of \text{SUBROUTINE DEBUGGING OFF}, \text{SUBROUTINE DEBUGGING ON}, \text{SUBROUTINE REAL
PARAMETER}, \text{SUBROUTINE INTEGER PARAMETER}, and \text{SUBROUTINE STRING PARAMETER}. Ex-
amples of using these command lines are provided throughout Chapter 9.

The magnitude set in the user subroutine can be scaled by use of the \text{SCALE FACTOR} command
line, as described in Section 6.5.2.4.

\textbf{Usage requirements for the node set subroutine.} The node set subroutine that you write will
return six values per node. Suppose you have written a user subroutine that passes the output
values through an array \text{output_values}. For a given node \text{inode}, the \text{output_values} array
would have the following values:

\[
\text{output_values(1,inode)} = \text{magnitude of traction}\]
\[
\text{output(values(2,inode)} = \text{not used}\]
\[
\text{output_values(3,inode)} = \text{not used}\]
\[
\text{output_values(4,inode)} = \text{x component of direction vector}\]
\[
\text{output_values(5,inode)} = \text{y component of direction vector}\]
\[
\text{output_values(6,inode)} = \text{z component of direction vector}\]

The direction in which the traction will act is given by components 4 through 6 of \text{output_values}
for \text{inode}. The magnitude of the traction in the specified direction is given by component 1 of
\text{output_values} at \text{inode}. The total force on each node is found by integrating the local nodal
tractions using the associated directions, which are normalized by Presto over the face areas. The
values of the flags array are not used.

See Chapter 9 for more details on implementing the user subroutine option.
6.5.2.4 Additional Commands

These command lines in the TRACTION command block provide additional options for the boundary condition:

```
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
```

The SCALE FACTOR command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the traction in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the traction from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The ACTIVE PERIODS command line determines when the boundary condition is active. See Section 2.5 for more information about this command line.
6.5.3 Prescribed Force

The PRESCRIBED FORCE command block prescribes a force field for a given set of nodes. The force field associates a vector giving the magnitude and direction of the force with each node in the node set. The force field may vary over time and space. If the force field has only a time-varying component, the specification commands in the above command block can be used to specify the force field. If the force field has both time-varying and spatially varying components, a user subroutine is used to specify the force field. You cannot use both the specification commands and the user subroutine commands in the same command block.

The PRESCRIBED FORCE command block contains three groups of commands—node set, function, and user subroutine. Each of these command groups is basically independent of the others. In addition to the command lines in the three command groups, there are two additional command lines: SCALE FACTOR and ACTIVE PERIODS. The SCALE FACTOR command line can be used in conjunction with either the specification commands or the user subroutine commands. The ACTIVE PERIODS command line is used to activate or deactivate this force boundary condition for certain time periods. Following are descriptions of the different command groups and the
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SCALE FACTOR and ACTIVE PERIODS command lines.

6.5.3.1 Node Set Commands

The \{node set commands\} portion of the PRESCRIBED FORCE command block defines a set of nodes associated with the prescribed force field and can include some combination of the following command lines:

- NODE SET = <string list>nodelist_names
- SURFACE = <string list>surface_names
- BLOCK = <string list>block_names
- INCLUDE ALL BLOCKS
- REMOVE NODE SET = <string list>nodelist_names
- REMOVE SURFACE = <string list>surface_names
- REMOVE BLOCK = <string list>block_names

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one NODE SET, SURFACE, BLOCK, or INCLUDE ALL BLOCKS command line in the command block.

6.5.3.2 Specification Commands

If the specification commands are used, the force vector at any given time is the same for all nodes in the node set associated with the particular PRESCRIBED FORCE command block. The direction of the force vector is constant for all time; the magnitude of the force vector may vary with time, however.

Following are the command lines used to specify the prescribe force with a direction and a function:

- DIRECTION = <string>defined_direction
- COMPONENT = <string>X|Y|Z
- FUNCTION = <string>function_name

The force can be specified either along an arbitrary user-defined direction or along a component direction (X, Y, or Z), but not both.

- The DIRECTION command line is used to prescribe force in an arbitrary user-defined direction. The name in the string defined_direction is a reference to a direction, which is defined using the DEFINE DIRECTION command block within the domain scope.

- The COMPONENT command line is used to specify that the force vector lies along one of the component directions. The COMPONENT command line is a shortcut to an internally defined direction vector; for example, component \( \times \) corresponds to using direction vector \( (1, 0, 0) \).
The magnitude of the force is specified by the FUNCTION command line. This references a function_name (defined in the domain scope in a DEFINITION FOR FUNCTION command block) that specifies the magnitude of the force vector as a function of time. The magnitude can be scaled by use of the SCALE FACTOR command line described in Section 6.5.3.4.

The force is applied only in the prescribed direction, and is not applied in any direction orthogonal to that direction.

### 6.5.3.3 User Subroutine Commands

If the user subroutine option is used, the force vector may vary spatially at any given time for each of the nodes in the node set associated with the particular PRESCRIBED FORCE command block. The user subroutine option allows for a more complex description of the force field than does the function option, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a force direction and a magnitude for every node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the force field.

Following are the command lines related to the user subroutine option:

```plaintext
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name = <string>param_value
```

The user subroutine option is invoked by using the NODE SET SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user.

Following the NODE SET SUBROUTINE command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 9.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided throughout Chapter 9.

The magnitude set in the user subroutine can be scaled by use of the SCALE FACTOR command line, as described in Section 6.5.3.4.

**Usage requirements for the node set subroutine.** The subroutine that you write will return three output values per node. Suppose you write a user subroutine that passes the output values through an array output_values. For a given node inode, the output_values array would have the following values:

```plaintext
output_values(1,inode) = x component of force at inode
```
output_values(2,inode) = y component of force at inode
output_values(3,inode) = z component of force at inode

The three components of the force vector are given in output_values 1 through 3. The values of the flags array are ignored.

See Chapter 9 for more details on implementing the user subroutine option.

6.5.3.4 Additional Commands

These command lines in the PRESCRIBED FORCE command block provide additional options for the boundary condition:

SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names

The SCALE FACTOR command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the force in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the force from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The ACTIVE PERIODS command line determines when the boundary condition is active. See Section 2.5 for more information about this command line.
6.5.4 Prescribed Moment

BEGIN PRESCRIBED MOMENT

# {node set commands}
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
#
# specification commands
DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z
FUNCTION = <string>function_name
#
# user subroutine commands
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
#
# additional commands
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
END [PRESCRIBED MOMENT]

The PRESCRIBED MOMENT command block prescribes a moment field for a given set of nodes. Moments can only be defined for nodes attached to beam or shell elements. The moment field associates a vector giving the magnitude and direction of the moment with each node in the node set. If the moment field has only a time-varying component, the specification commands in the above command block can be used to specify the moment field. If the moment field has both time-varying and spatially varying components, a user subroutine option is used to specify the moment field. You cannot use both the specification commands and the user subroutine commands in the same command block.

The PRESCRIBED MOMENT command block contains three groups of commands—node set, function, and user subroutine. Each of these command groups is basically independent of the others. In addition to the command lines in the three command groups, there are two additional command lines: SCALE FACTOR and ACTIVE PERIODS. The SCALE FACTOR command line can be used in conjunction with either the specification commands or the user subroutine commands. The ACTIVE PERIODS command line is used to activate or deactivate this force boundary condi-
tion for certain time periods. Following are descriptions of the different command groups and the SCALE FACTOR and ACTIVE PERIODS command lines.

6.5.4.1 Node Set Commands

The {node set commands} portion of the PRESCRIBED MOMENT command block defines a set of nodes associated with the prescribed moment field and can include some combination of the following command lines:

NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one NODE SET, SURFACE, BLOCK, or INCLUDE ALL BLOCKS command line in the command block.

6.5.4.2 Specification Commands

If the specification commands are used, the moment vector at any given time is the same for all nodes in the node set associated with the particular PRESCRIBED MOMENT command block. The direction of the moment vector is constant for all time; the magnitude of the moment vector may vary with time, however.

Following are the command lines used to specify the prescribed moment with a function and a direction:

DIRECTION = <string>defined_direction |
COMPONENT = <string>X|Y|Z
FUNCTION = <string>function_name

The moment can be specified either along an arbitrary user-defined direction or along a component direction (X, Y, or Z), but not both.

- The DIRECTION command line is used to prescribe the moment in an arbitrary user-defined direction. The name in the string defined_direction is a reference to a direction, which is defined using the DEFINE DIRECTION command block within the domain scope.

- The COMPONENT command line is used to specify that the moment vector lies along one of the component directions. The COMPONENT command line is a shortcut to an internally defined direction vector; for example, component x corresponds to using direction vector (1, 0, 0).
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The magnitude of the moment is specified by the FUNCTION command line. This references a function_name (defined in the domain scope in a DEFINITION FOR FUNCTION command block) that specifies the magnitude of the moment vector as a function of time. The magnitude can be scaled by use of the SCALE FACTOR command line described in Section 6.5.4.4.

The moment is applied only in the prescribed direction, and is not applied in any direction orthogonal to that direction.

6.5.4.3 User Subroutine Commands

If the user subroutine option is used, the moment vector may vary spatially at any given time for each of the nodes in the node set associated with the particular PRESCRIBED MOMENT command block. The user subroutine option allows for a more complex description of the moment field than do specification commands, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a moment direction and a magnitude for every node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the moment field.

Following are the command lines related to the user subroutine option:

- NODE SET SUBROUTINE = <string>subroutine_name
- SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
- SUBROUTINE REAL PARAMETER: <string>param_name = <real>param_value
- SUBROUTINE INTEGER PARAMETER: <string>param_name = <integer>param_value
- SUBROUTINE STRING PARAMETER: <string>param_name = <string>param_value

The user subroutine option is invoked by using the NODE SET SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user.

Following the NODE SET SUBROUTINE command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 9.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided throughout Chapter 9.

The magnitude set in the user subroutine can be scaled by use of the SCALE FACTOR command line, as described in Section 6.5.4.4.

Usage requirements for the node set subroutine. The subroutine that you write will return three output values per node. Suppose you write a user subroutine that passes the output values through an array output_values. For a given node inode, the output_values array would have the following values:

\[
\text{output_values}(1, \text{inode}) = \text{moment about x-direction at inode}
\]
6.6. GRAVITY

output_values(2,inode) = moment about y-direction at inode
output_values(3,inode) = moment about z-direction at inode

The three components of the moment vector are given in output_values 1 through 3. The values of the flags array are ignored.

See Chapter 9 for more details on implementing the user subroutine option.

6.5.4.4 Additional Commands

These command lines in the PRESCRIBED MOMENT command block provide additional options for the boundary condition:

SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names

The SCALE FACTOR command line is used to apply an additional scaling factor, which is constant in both time and space, to all vector magnitude values of the field defined by the specification commands or the user subroutine. For example, if the magnitude of the moment in a time history function is given as 1.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the magnitude of the moment from time 1.0 to 2.0 is 0.75. The default value for the scale factor is 1.0.

The ACTIVE PERIODS command line determines when the boundary condition is active. See Section 2.5 for more information about this command line.

6.6 Gravity

BEGIN GRAVITY

# {node set commands}
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
#
DIRECTION = <string>defined_direction
FUNCTION = <string>function_name
GRAVITATIONAL CONSTANT = <real>g_constant
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
END [GRAVITY]

A gravity load is generally referred to as a body force boundary condition. A gravity load generates a force at a node that is proportional to the mass of the node. This section describes how to apply a gravity load to a body.
The **GRAVITY** command block is used to specify a gravity load that is applied to all nodes selected within a command block. The gravity load boundary condition uses the function and scale (gravitational constant and scale factor) information to generate a body force at a node based on the mass of the node. Multiple **GRAVITY** command blocks can be defined on different sets of nodes. If two different **GRAVITY** command blocks reference the same node, the node will have gravity loads applied by both of the command blocks. Care must be taken to make sure you do not apply multiple gravity loads to one block if you only want one gravity load condition applied.

The **{node set commands}** portion of the **GRAVITY** command block defines a set of nodes associated with the gravity load and can include some combination of the following command lines:

```plaintext
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one **NODE SET**, **SURFACE**, **BLOCK**, or **INCLUDE ALL BLOCKS** command line in the command block.

The gravity load is specified along an arbitrary user-defined direction, and is defined using the **DIRECTION** command line. The name in the string *defined_direction* is a reference to a direction, which is defined using the **DEFINE DIRECTION** command block within the domain scope.

The strength of the gravitational field can be varied with time by using the **FUNCTION** command line. This command line references a *function_name* defined in the domain scope in a **DEFINITION FOR FUNCTION** command block.

A gravitational constant is specified by the **GRAVITATIONAL CONSTANT** command line in the real value *g_constant*. For example, the gravitational constant in units of inches and seconds would be 386.4 inches per second squared. You must set this quantity based on the actual units for your model.

The dependent variables in the function can be scaled by the real value *scale_factor* in the **SCALE FACTOR** command line. At any given time, the strength of the gravitational field is a product of the gravitational constant, the value of the function at that time, and the scale factor.

The **ACTIVE PERIODS** command line provides an additional option for the gravity load condition. This command line can activate or deactivate the gravity load for certain time periods. See Section 2.5 for more information about this command line.
6.7 Prescribed Temperature

BEGIN PRESCRIBED TEMPERATURE
   # {block set commands}
   BLOCK = <string list>block_names
   INCLUDE ALL BLOCKS
   REMOVE BLOCK = <string list>block_names
   #
   # specification command
   FUNCTION = <string>function_name
   #
   # user subroutine commands
   NODE SET SUBROUTINE = <string>subroutine_name
   SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
   SUBROUTINE REAL PARAMETER: <string>param_name
      = <real>param_value
   SUBROUTINE INTEGER PARAMETER: <string>param_name
      = <integer>param_value
   SUBROUTINE STRING PARAMETER: <string>param_name
      = <string>param_value
   #
   # read variable commands
   READ VARIABLE = <string>variable_name
   TIME = <real>time
   #
   # additional commands
   SCALE FACTOR = <real>scale_factor(1.0)
   ACTIVE PERIODS = <string list>period_names
END [PRESCRIBED ACCELERATION]

The PRESCRIBED TEMPERATURE command block prescribes a temperature field for a given set of nodes. The prescribed temperature is for each node in the node set. The temperature field may vary over time and space. If the temperature field has only a time-varying component, the function command in the above command block can be used to specify the temperature field. If the temperature field has both time-varying and spatially varying components, a user subroutine option can be used to specify the temperature field. Finally, you may also read the temperature as a variable from the mesh file. You can select only one of these options—function, user subroutine, or read variable—in a command block.

Temperature is applied to nodes, but it is frequently used at the element level, such as in the case for thermal strains. If the temperatures are used at the element level, the nodal values are averaged (depending on element) connectivity to produce an element temperature. The temperatures must be defined for all the nodes defining the connectivity for any given element. For this reason, we use block commands to derive a set of nodes at which to define temperatures. If the temperatures are used on an element basis, then the temperature at all the necessary nodes will be defined.

The PRESCRIBED TEMPERATURE command block contains four groups of commands—block set,
function, user subroutine, and read variable. Each of these command groups is basically independent of the others. In addition to the command lines in the four command groups, there are two additional command lines: SCALE FACTOR and ACTIVE PERIODS. The SCALE FACTOR command line can be used in conjunction with the function command, the user subroutine option, or the read variable option. The ACTIVE PERIODS command line is used to activate or deactivate this kinematic boundary condition for certain time periods. Following are descriptions of the different command groups and the SCALE FACTOR and ACTIVE PERIODS command lines.

### 6.7.1 Block Set Commands

The block set commands portion of the PRESCRIBED TEMPERATURE command block defines a set of nodes associated with the prescribed temperature field and can include some combination of the following command lines:

```
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes derived from some combination of element blocks. See Section 6.1.1 for more information about the use of these command lines for creating a set of nodes used by the boundary condition. There must be at least one BLOCK or INCLUDE ALL BLOCKS command line in the command block.

### 6.7.2 Specification Command

If the function command is used, the temperature at any given time is the same for all nodes in the node set associated with the particular PRESCRIBED TEMPERATURE command block. The command line

```
FUNCTION = <string>function_name
```

references a function_name (defined in the domain scope using a DEFINITION FOR FUNCTION command block) that specifies the temperature as a function of time. The temperature can be scaled by use of the SCALE FACTOR command line described in Section 6.7.5.

### 6.7.3 User Subroutine Commands

If the user subroutine option is used, the temperature field may vary spatially at any given time for each of the nodes in the node set associated with the particular PRESCRIBED TEMPERATURE command block. The user subroutine option allows for a more complex description of the temperature field than does the function command, but the user subroutine option also requires that you write a user subroutine to implement this capability. The user subroutine will be used to define a
temperature for every node to which the boundary condition will be applied. The subroutine will be called by Presto at the appropriate time to generate the temperature field.

Following are the command lines related to the user subroutine option:

```plaintext
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name = <string>param_value
```

The user subroutine option is invoked by using the `NODE SET SUBROUTINE` command line. The string `subroutine_name` is the name of a FORTRAN subroutine that is written by the user.

Following the `NODE SET SUBROUTINE` command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 9.2.2 and consist of `SUBROUTINE DEBUGGING OFF`, `SUBROUTINE DEBUGGING ON`, `SUBROUTINE REAL PARAMETER`, `SUBROUTINE INTEGER PARAMETER`, and `SUBROUTINE STRING PARAMETER`. Examples of using these command lines are provided throughout Chapter 9.

The temperature set in the user subroutine can be scaled by use of the `SCALE FACTOR` command line, as described in Section 6.7.5.

See Chapter 9 for more details on implementing the user subroutine option.

### 6.7.4 Read Variable Commands

If the read variable option is used, the temperature field will be read from a variable defined in the mesh file. The following command lines are used for the read variable option:

```plaintext
READ VARIABLE = <string>mesh_var_name
TIME = <real>temp_time
```

The string `mesh_var_name` must correspond to the variable name for the temperature field present in the mesh file. The temperature field may be specified at several different times on the mesh file. You may select the temperature field at a specific time by using the `TIME` command line. If the specified time on the `TIME` command line does not correspond exactly to a time on the mesh file, the data on the mesh file will be interpolated as needed to obtain the nodal temperatures.

The temperature set by the read variable option can be scaled by use of the `SCALE FACTOR` command line, as described in Section 6.7.5.
6.7.5 Additional Commands

These command lines in the PRESCRIBED TEMPERATURE command block provide additional options for the boundary condition:

```
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
```

The SCALE FACTOR command line is used to apply an additional scaling factor, which is constant in both time and space, to all temperature values of the field defined by the function command, the user subroutine, or the read variable option. For example, if the temperature in a time history function is given as 100.5 from time 1.0 to time 2.0 and the scale factor is 0.5, then the temperature from time 1.0 to 2.0 is 50.25. The default value for the scale factor is 1.0.

The ACTIVE PERIODS command line determines when the boundary condition is active. See Section 2.5 for more information about this command line.
6.8 Specialized Boundary Conditions

There are a number of specialized boundary conditions implemented in Presto. Some of them enforce kinematic conditions, and some result in the application of loads.
6.8.1 Cavity Expansion

BEGIN CAVITY EXPANSION
   EXPANSION RADIUS = <string>SPHERICAL|CYLINDRICAL
   (spherical)
   SURFACE = <string list>surface_ids
   REMOVE SURFACE = <string list>surface_ids
   FREE SURFACE = <real>top_surface_zcoord
                   <real>bottom_surface_zcoord
   NODE SETS TO DEFINE BODY AXIS =
      <string>nodelist_1 <string>nodelist_id2
   TIP RADIUS = <real>tip_radius
   BEGIN LAYER <string>layer_name
      LAYER SURFACE = <real>top_layer_zcoord
                   <real>bottom_layer_zcoord
      PRESSURE COEFFICIENTS = <real>c0 <real>c1 <real>c2
      SURFACE EFFECT = <string>NONE|SIMPLE_ON_OFF(NONE)
      FREE SURFACE EFFECT COEFFICIENTS = <real>coeff1
                                       <real>coeff2
   END [LAYER <string>layer_name]
   ACTIVE PERIODS = <string list>period_names
END [CAVITY EXPANSION]

The CAVITY EXPANSION command block is used to apply a cavity expansion boundary condition to a surface on a body. This boundary condition is typically used for earth penetration studies where some type of projectile (penetrator) strikes a target. For a more detailed explanation of the numerical implementation of the cavity expansion boundary condition and the parameters for this boundary condition, consult Reference 1. The cavity expansion boundary condition is a complex boundary condition with several options, and the detailed explanation of the implementation of the boundary condition in the above reference is required reading to fully understand the input parameters for this boundary condition.

There are two types of cavity expansion—cylindrical expansion and spherical expansion. You can select either the spherical or cylindrical option by using the EXPANSION RADIUS command line; the default is SPHERICAL. Reference 1 describes these two types of cavity expansion.

The boundary condition is applied to the surfaces (surface_ids) in the finite element model specified by the SURFACE command line. (Any surface specified on the SURFACE command line can be removed from the list of surfaces by using a REMOVE SURFACE command line.) This boundary condition generates a pressure at a node based on the velocity and surface geometry at the node. Since cavity expansion is essentially a pressure boundary condition, cavity expansion must be specified for a surface.

The target has a top free surface with a normal in the global positive z-direction; the target has a bottom free surface with a normal in the global negative z-direction. The point on the global z-axis intersected by the top free surface is given by the parameter top_surface_zcoord on the FREE SURFACE command line. The point on the global z-axis intersected by the bottom free surface is given by the parameter bottom_surface_zcoord on the FREE SURFACE command
6.8. *SPECIALIZED BOUNDARY CONDITIONS*

It is necessary to define two points that lie on the axis (usually the axis of revolution) of the penetrator. These two nodes are specified with the **NODE SETS TO DEFINE BODY AXIS** command line. The first node should be a node toward the tip of the penetrator \( (\text{nodelist}_1) \), and the second node should be a node toward the back of the penetrator \( (\text{nodelist}_2) \). Only one node is allowed in each node set.

It is necessary to compute either a spherical or cylindrical radius for nodes on the surface where the cavity expansion boundary condition is applied. This is done automatically for most nodes. The calculations for these radii break down if the node is close to or at the tip of the axis of revolution of the penetrator. For nodes where the radii calculations break down, a user-defined radius can be specified with the **TIP RADIUS** command line. For more information, consult Reference 1.

Embedded within the target can be any number of layers. Each layer is defined with a **LAYER** command block. The command block begins with

```
BEGIN LAYER <string>layer_name
```

and is terminated with:

```
END [LAYER <string>layer_name]
```

Here the string `layer_name` is a user-selected name for the layer. This name must be unique to all other layer names defined in the **CAVITY EXPANSION** command blocks. The layer properties are defined by several different command lines—**LAYER SURFACE**, **PRESSURE COEFFICIENTS**, **SURFACE EFFECT**, and **FREE SURFACE EFFECT COEFFICIENTS**. These command lines are described next.

- **LAYER SURFACE** = <real>top_layer_zcoord
  <real>bottom_layer_zcoord

  The layer has a top surface with a normal in the global positive \( z \)-direction; the layer has a bottom surface with a normal in the global negative \( z \)-direction. In the **LAYER SURFACE** command line, the point on the global \( z \)-axis intersected by the top layer surface is given by the parameter `top_layer_zcoord`, and the point on the global \( z \)-axis intersected by the bottom layer surface is given by the parameter `bottom_layer_zcoord`.

- **PRESSURE COEFFICIENTS** = <real>c0 <real>c1 <real>c2

  The value of the pressure at a node is derived from an equation that is quadratic based on some scalar value derived from the velocity vector at the node. The three coefficients for the quadratic equation \( (c0, c1, c2) \) in the **PRESSURE COEFFICIENTS** command line define the impact properties of a layer.

- **SURFACE EFFECT** = <string>NONE|SIMPLE_ON\str (NONE)

  There can be no surface effects associated with a layer, or there can be a simple on/off surface effect model associated with a layer. The type of surface effect is determined by the **SURFACE EFFECT** command line. The default is no surface effects. If the **SIMPLE_ON_OFF** model is chosen, it is necessary to specify free surface effect coefficients with the **FREE SURFACE EFFECT COEFFICIENTS** command line.
- FREE SURFACE EFFECT COEFFICIENTS = <real>coeff1 <real>coeff2

All the parameters defined in a LAYER command block apply to that layer. If a simple on/off surface effect is applied to a layer, the surface effect coefficients are associated with the layer values. The surface effect parameter associated with the top of the layer is coeff1; the surface effect parameter associated with the bottom of the layer is coeff2.

The ACTIVE PERIODS command line provides an additional option for cavity expansion. This command line can activate or deactivate cavity expansion for certain time periods. See Section 2.5 for more information about this command line.
6.8. SPECIALIZED BOUNDARY CONDITIONS

6.8.2 Silent Boundary

BEGIN SILENT BOUNDARY
  SURFACE = <string list>surface_names
  REMOVE SURFACE = <string list>surface_names
  ACTIVE PERIODS = <string list>period_names
END [SILENT BOUNDARY]

The SILENT BOUNDARY command block is also referred to as a non-reflecting surface boundary condition. A wave striking this surface is not reflected. This boundary condition is implemented with the techniques described in Reference 2. The method described in this reference is excellent at transmitting the low- and medium-frequency content through the boundary. While the method does reflect some of the high-frequency content, the amount of energy reflected is usually minimal. On the whole, the silent boundary condition implemented in Presto is highly effective.

In the SURFACE command line, you can list a series of surfaces through the string list surface_names. There must be at least one SURFACE command line in the command block. The REMOVE SURFACE command line allows you to delete surfaces from the set specified in the SURFACE command line(s) through the string list surface_names. See Section 6.1.1 for more information about the use of these command lines for creating a set of surfaces used by the boundary condition.

The ACTIVE PERIODS command line provides an additional option for the boundary condition. This command line is used to activate or deactivate the boundary condition for certain time periods. See Section 2.5 for more information about this command line.
### 6.8.3 Spot-Weld

The spot-weld option lets the user model an “attachment” between a node on one surface and a face on another surface. This option models a weld or a small screw or bolt with a normal force-displacement curve like that shown in Figure 6.1 and a tangential force-displacement curve like that shown in Figure 6.2. The displacement shown in the figures is the distance, either normal or tangential, that the node moves from the nearest point on the face as measured in the original configuration. The force shown in the figure is the force at the attachment as a function of the distance between the two attachment points. (The force-displacement curve assumes the two attachment points are originally at the same location and the initial distance is zero, thus zero force at time zero. However, in most situations there is an initial gap which leads to non-zero forces at time zero.) Two force-displacement curves are required for the spot-weld model; one curve models normal behavior, and the other curve models tangential behavior. It is worth noting the difference in how the normal and tangential components behave, therefore explaining why two curves are required. It is possible for the node to interpenetrate the surface resulting in a negative normal displacement between the connection points. Therefore, the normal force displacement curve must have the ability to capture negative displacements and thus negative forces. Although this penalty stiffness approach will work to prevent interpenetration, it is better to model this behavior using contact. The tangential displacement is always positive because there is no decent way to define positive and negative displacements that are tangential to the surface.

The attachment in Presto is defined between a node on one surface and the closest point on an element face on the other surface. Since a face is used to define one of the attachment points, it is possible to compute a normal vector and a tangent vector associated with the face. This allows us to resolve the displacement (distance, both positive and negative) and force (both tensile
and compressive) into normal and tangential components. With normal and tangential vectors associated with the attachment, the attachment can be characterized for the case of pure tension and pure shear.

Presto includes two mechanisms for determining failure for cases that fall between pure tension and pure shear. In the first case, failure is governed by the equation

\[(u_n/u_{n\text{crit}})^p + (u_t/u_{t\text{crit}})^p < 1.0.\]  \hspace{1cm} (6.1)

In Equation 6.1, the distance from the node to the original attachment point on the face as measured normal to the face is \(u_n\), which is defined as the normal distance. The maximum value given for \(u_n\) in the normal force-displacement curve is \(u_{n\text{crit}}\), but is different for positive and negative displacements. The distance from the node to the original attachment point on the face as measured along a tangent to the face is \(u_t\), which is defined as the tangential distance. The maximum value given for \(u_t\) in the tangential force-displacement curve is \(u_{t\text{crit}}\), but is different for positive and negative displacements. In Figure 6.1, the maximum value for the displacement is \(u_{\text{crit}+}\) in the positive direction and \(u_{\text{crit}-}\) in the negative direction. The value \(p\) is a user-specified exponent that controls the shape of the failure surface.

Alternatively, Presto permits a user-specified function to determine the failure surface. The function defines the ratio of \(u_t/u_{t\text{crit}}\) at which failure will occur as a function of \(u_n/u_{n\text{crit}}\). The function must range from 0.0 to 1.0, and have a value of 1.0 at 0.0 and a value of 0.0 at 1.0. These restrictions
CHAPTER 6. BOUNDARY CONDITIONS AND INITIAL CONDITIONS

Figure 6.2: Force-displacement curve for spot-weld tangential force.

preserve proper failure for the cases of pure tension and pure shear.

To use the spot-weld option in Presto, a SPOT WELD command block begins with the input line:

BEGIN SPOT WELD

and is terminated with the input line:

END [SPOT WELD]

Within the command block, it is necessary to specify the set of nodes on one side of the spot-weld with the NODE SET command line. The NODE SET command line can list one or more node sets. Any node set listed on the NODE SET command line can be deleted from the list of node sets by using a REMOVE NODE SET command line. A set of element faces on an opposing side of the spot-weld (which we will refer to as the first surface) is specified with the SURFACE command line. The SURFACE command line can list one or more surfaces. Any surface listed on the SURFACE command line can be deleted from the list of surfaces by using a REMOVE SURFACE command line. For any node in the node set, the closest point to this node on the opposing surface should lie within the element faces specified by the SURFACE command line.

The normal force-displacement curve is specified by a function named by the value function_nor_disp in the NORMAL DISPLACEMENT FUNCTION command line. This function can be scaled by the real value scale_nor_disp in the NORMAL DISPLACEMENT SCALE FACTOR command line; the default for this factor is 1.0. The tangential force-displacement curve is specified by a function named by the string function_tang_disp in the TANGENTIAL DISPLACEMENT FUNCTION command line. This function can be scaled by the real value scale_tang Disp given in the TANGENTIAL DISPLACEMENT SCALE FACTOR command line; the default for this factor is 1.0.

The failure surface between pure tension and pure shear is controlled by specifying either the failure envelope exponent, $p$ in Equation 6.1, or a failure function. The failure exponent is specified by the real value exponent in the FAILURE ENVELOPE EXPONENT command line. The failure function is specified by the FAILURE FUNCTION command line. If both a failure function and a
failure exponent are given, then the failure function is used.

For an explicit, transient dynamics code like Presto, it is better to remove the force for the spot-weld over several load steps rather than over a single load step once the failure criterion is exceeded. The FAILURE DECAY CYCLES command line controls the number of load steps over which the final force is removed (default value is 10). To remove the final force at a spot-weld over five load increments, the integer specified by number_decay_cycles would be set to 5. Once the force at the spot-weld is reduced to zero, it remains zero for all subsequent time (despite the function definition).

The spot-weld can take on area-based behavior by specifying a surface in place of a set of nodes. The identifier of this surface is specified by the string surface_id in the SECOND SURFACE command line. The area-based spot-weld creates a weld between all nodes on the second surface and the faces of the first surface. The load-resistance curve at each node is derived from the tributary area of the node times the given force-displacement curves. Thus, for the area-based spot-welds, the force-displacement curves give the force per unit area resisted by the weld.

The user must set a tolerance for the node-to-face search with the

    SEARCH TOLERANCE = <real>search_tolerance

command line. The value you select for search_tolerance will depend upon the distance between the nodes and surfaces used to define the spot-weld.

If the user sets IGNORE INITIAL OFFSET = YES, the initial offset vector between the node and the surface will be used as a relative zero displacement, which allows a spot weld to initially have zero force even if there are small separations a priori.

The ACTIVE PERIODS command line provides an additional option for the boundary condition. This command line is used to activate or deactivate the boundary condition for certain time periods. See Section 2.5 for more information about this command line.

Output data can be obtained from spot welds. The list of available output variables is documented in Table 8.16.
6.8.4 Line Weld

BEGIN LINE WELD
  SURFACE = <string list> surface_names
  REMOVE SURFACE = <string list> surface_names
  BLOCK = <string list> block_names
  REMOVE BLOCK = <string list> block_names
  SEARCH TOLERANCE = <real> search_tolerance
  R DISPLACEMENT FUNCTION = <string> r_disp_function_name
  R DISPLACEMENT SCALE FACTOR = <real> r_disp_scale
  S DISPLACEMENT FUNCTION = <string> s_disp_function_name
  S DISPLACEMENT SCALE FACTOR = <real> s_disp_scale
  T DISPLACEMENT FUNCTION = <string> t_disp_function_name
  T DISPLACEMENT SCALE FACTOR = <real> t_disp_scale
  R ROTATION FUNCTION = <string> r_rotation_function_name
  R ROTATION SCALE FACTOR = <real> r_rotation_scale
  S ROTATION FUNCTION = <string> s_rotation_function_name
  S ROTATION SCALE FACTOR = <real> s_rotation_scale
  T ROTATION FUNCTION = <string> t_rotation_function_name
  T ROTATION SCALE FACTOR = <real> t_rotation_scale
  FAILURE ENVELOPE EXPONENT = <real> k
  FAILURE DECAY CYCLES = <integer> number_decay_cycles
  ACTIVE PERIODS = <string list> period_names
END LINE WELD

The line-weld capability is used to weld the edge of a shell to the face of another shell. The bond can transmit both translational and rotational forces. When failure of the line weld occurs, it breaks and no longer transmits any forces.

The edge of the shell that is tied to a surface is modeled with a block of one-dimensional elements (truss, beam, spring, etc.). The edge of the shell and the one-dimensional elements will share the same nodes. We will refer to the shell edge and the one-dimensional elements associated with it as the one-dimensional part of the line-weld model. The element blocks with the one-dimensional elements are specified by using the BLOCK command line. More than one element block can be listed on this command line. The element blocks referenced by the BLOCK command line must be one-dimensional elements—truss, beam, spring, etc.

The other part of the line weld is a set of faces defined by shell elements; this set of faces is the two-dimensional part of the line weld. The surface (the two-dimensional part of the model) to which the nodes (from the one-dimensional part of the model) are to be bonded is defined by any surface of element faces derived from shell elements. The line weld will bond each node in the element blocks listed in the BLOCK command line to the closest face (or faces) of element faces in the surfaces listed in the SURFACE command line. More than one surface can be listed on this command line.

The command line SEARCH TOLERANCE sets a tolerance on the search for node-to-face interactions. For a given node, only those faces within the distance set by the search_tolerance parameter will be searched to determine whether the node should be welded to the face.
6.8. SPECIALIZED BOUNDARY CONDITIONS

Each section of the line weld has its own local coordinate system \((r, s, t)\). The \(r\)-direction lies along a one-dimensional element (and hence on the surface). The \(s\)-direction lies on the surface and is tangential to the one-dimensional element. The \(t\)-direction lies normal to the face and is orthogonal to the \(r\)- and \(s\)-directions. Force-displacement functions and moment-rotation functions may be specified for all axes in the local coordinate system. If one of the functions is left out, the resistance is zero for that axis. These functions are similar to the ones used for the spot-weld (see Figure 6.2).

The force-displacement function in the \(r\)-direction represents shear resistance in the direction of the weld; this function is specified by a SIERRA function name on the \texttt{R DISPLACEMENT FUNCTION} command line. The force-displacement in the \(s\)-direction represents shear resistance tangential to the weld; this function is specified by a SIERRA function name on the \texttt{S DISPLACEMENT FUNCTION} command line. The force-displacement in the \(t\)-direction function represents tearing resistance normal to the surface; this function is specified by a SIERRA function name on the \texttt{T DISPLACEMENT FUNCTION} command line. The moment-rotation about the \(r\)-axis represents a rotational tearing resistance; this is specified by a SIERRA function name on the \texttt{R ROTATION FUNCTION} command line. The rotational resistances about the \(s\)-direction and the \(t\)-direction are likely not very meaningful, as rotations along these axes should be well constrained by the normal and tangential displacement relations. These two rotational resistances, if used, are defined with SIERRA function names on the \texttt{S ROTATION FUNCTION} and \texttt{T ROTATION FUNCTION} command lines. Note that each SIERRA function used in this command block is defined via a \texttt{DEFINITION FOR FUNCTION} command block in the domain scope.

Any of the above functions can be scaled by using a corresponding scale factor. For example, the force-displacement function on the \texttt{R DISPLACEMENT FUNCTION} command line can be scaled by the parameter \(r\_disp\_scale\) on the \texttt{R DISPLACEMENT SCALE FACTOR} command line. Only the force values of the force-displacement curve will be scaled.

The failure function for the line weld is similar to that for the spot-weld. Denote the displacement or rotation associated with a line weld as \(\delta\). Suppose that \(\delta_i\) is a displacement in the \(r\)-direction. The force-displacement curve specified on the \texttt{R DISPLACEMENT FUNCTION} command line has a maximum value \(\eta\). This is the maximum displacement the weld can endure in the \(r\)-direction before breaking. Associate this value of \(\eta\) with \(\delta_i\) by designating it as \(\eta_i\). Repeat this pairing process for all the displacements and rotations defining the line weld. Each displacement component in the line weld will be paired with one of the three maximum displacement values associated with the line weld. Each rotation component in the line weld will be paired with one of the three maximum rotation values associated with the line weld. Breaking of the weld under combined loading is calculated the same as the spot-weld. The weld breaks if

\[
\sqrt{k \sum \left( \frac{\delta_i}{\eta_i} \right)^k} > 1.
\]  
(6.2)

In the above equation, the parameter \(k\) is set by the user. A typical value for \(k\) is 2. The summation takes place over all the failure functions (force-displacement and moment-rotation) for all the nodes. (The value for \(k\) is specified on the \texttt{FAILURE ENVELOPE EXPONENT} command line.)
For an explicit, transient dynamics code like Presto, it is better to remove the forces for the line weld over several time steps rather than over a single time step once the failure criterion is exceeded. The **FAILURE DECAY CYCLES** command line controls the number of time steps over which the final force is removed. To remove the final force at a line weld over five time steps, the integer specified by `number_decay_cycles` would be set to 5. Once the force in the line weld is reduced to zero, it remains zero for all subsequent time.

The **ACTIVE PERIODS** command line provides an additional option for the boundary condition. This command line is used to activate or deactivate the boundary condition for certain time periods. See Section 2.5 for more information about this command line.
6.8.5 Viscous Damping

BEGIN VISCOUS DAMPING <string>damp_name
# {block set commands}
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE BLOCK = <string list>block_names
#
MASS DAMPING COEFFICIENT = <real>mass_damping
STIFFNESS DAMPING COEFFICIENT = <real>stiff_damping
#
# additional command
ACTIVE PERIODS = <string list>period names
END [VISCOUS DAMPING <string>damp_name]

The VISCOUS DAMPING command block adds simple Rayleigh viscous damping to mesh nodes. At each node, Presto computes a damping coefficient, which is then multiplied by the node velocity to create a damping force. The damping coefficient is the sum of the mass times a mass damping coefficient and the nodal stiffness times a stiffness damping coefficient. In general, the mass damping portion damps out low-frequency modes in the mesh, while the stiffness damping portion damps out higher-frequency terms. Appropriate values for the damping coefficients depend on the frequencies of interest in the mesh. The general expression for the critical damping fraction, $c_d$, for a given frequency is

$$ c_d = \frac{k_d \omega + m_d / \omega}{2}, $$(6.3)

where $k_d$ is the stiffness damping coefficient, $m_d$ is the mass damping coefficient, and $\omega$ is the frequency of interest. The stiffness damping portion must be used with caution. Because this term depends on the stiffness, it can affect the critical time step. Thus certain ranges of values for the stiffness damping coefficient can change the critical time step for the mesh. As Presto does not currently modify the critical time step based on the selected values for this coefficient, some choices for this parameter can cause solution instability.

6.8.5.1 Block Set Commands

The {block set commands} portion of the VISCOUS DAMPING defines a set of element blocks associated with the viscous damping and can include some combination of the following command lines:

BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE BLOCK = <string list>block_names

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of element blocks. See Section 6.1.1 for more information about the use of these command lines for creating a set of element blocks used by viscous damping. There must be at least one BLOCK or INCLUDE ALL BLOCKS command line in the command block.
All the nodes associated with the elements specified by the block set commands will have viscous damping forces applied.

### 6.8.5.2 Viscous Damping Coefficient

The mass damping coefficient in Equation 6.3, \( m_d \), is specified using the parameter `mass_damping` on the command line:

\[
\text{MASS DAMPING COEFFICIENT} = \text{<real>mass_damping}
\]

Mass damping most strongly damps the low-frequency modes.

The stiffness damping coefficient command line in Equation 6.3, \( k_d \), is specified as the parameter `stiff_damping` on the command line:

\[
\text{STIFFNESS DAMPING COEFFICIENT} = \text{<real>stiff_damping}
\]

Stiffness damping most strongly damps high-frequency modes. Large values for the stiffness damping coefficient can affect the critical time step. Since Presto does not modify the critical time step based on the stiffness damping coefficient, it may be necessary for the user to manually decrease the critical time step.

### 6.8.5.3 Additional Command

The `ACTIVE PERIODS` command line can optionally appear in the `VISCOUS DAMPING` command block:

\[
\text{ACTIVE PERIODS} = \text{<string list>period_names}
\]

This command line can activate or deactivate the viscous damping for certain time periods. See Section 2.5 for more information about this command line.
6.8.6 Volume Repulsion Old

BEGIN VOLUME REPULSION OLD <string>repulsion
FRICITION COEFFICIENT = <real>fric_coeff
SCALE FACTOR = <real>scale_factor
OVERLAP TYPE = [NODAL|VOLUMETRIC]

BEGIN BLOCK SET <string>set
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE BLOCK = <string list>block_names
  #
  SURFACE = <string list>surface_names
  REMOVE SURFACE = <string list>surface_names
  #
  ACTIVE PERIODS = <string list>period names
  INACTIVE PERIODS = <string list>period names
  #
  LINE CYLINDER RADIUS = <real>cylinder_radius
  ELEMENT REPRESENTATION = [BEAM_ELEMENT_CYLINDERS|
                             TRUE_SOLID_VOLUME|NODES]
END [BLOCK SET <string>set]
END [VOLUME REPULSION OLD <string>repulsion]

The VOLUME REPULSION OLD command block is used to create a cylindrical volume around beam elements that is used as a frictional contact surface. Because beam elements are represented as line elements, there is no volume associated with the elements that can be used for contact. This command will generate nodal forces based on interpenetrations of a prescribed set of nodes with the cylindrical contact surfaces. The force is generated using a penalty stiffness method where the magnitude of the force depends on the mass of the node and the current time step. This command will be replaced by DASH contact in the future.

Definition of the coefficient of friction for the cylindrical surface is defined through the FRICITION COEFFICIENT command line.

The SCALE FACTOR command line specifies a scale factor that scales the force produced from node-surface interactions.

The OVERLAP TYPE command line must always be set to VOLUMETRIC.

6.8.6.1 Block Set

Complete definition of the contact surfaces and node sets are completely defined within multiple BLOCK SET command blocks. At least two BLOCK SET command blocks must be defined, one that defines the beam element blocks to wrap in cylinders by setting the ELEMENT REPRESENTATION command line to BEAM_ELEMENT_CYLINDERS. The second BLOCK SET command block defines the node set used to contact the cylindrical surfaces by setting the ELEMENT
The BLOCK, INCLUDE ALL BLOCKS and REMOVE BLOCK command lines must be used when defining the beam element blocks, while a combination of these block command lines and the following surface command lines, SURFACE and REMOVE SURFACE, must be used to define the node set used for contact.

ACTIVE PERIODS command line defined the time periods in which this boundary condition is active where as the INACTIVE PERIODS command line defines when this boundary condition is inactive.

The LINE CYLINDER RADIUS command line specifies the radius of the cylindrical surface around the beam elements.
6.9 References


Chapter 7

Contact

This chapter describes the input syntax for defining interactions of contact surfaces in a Presto analysis. For more information on contact and its computational details, consult References 1 and 2.

Contact refers to the interaction of one or more bodies when they physically touch. This can include the interaction of one part of a surface against another part of the same surface, the surface of one body against the surface of another body, and so forth. The contact algorithms within Presto are designed to ensure that surfaces do not inter-penetrate in a nonphysical way, and that the interface behavior is computed correctly according to any user-specified surface-physics models (e.g., energy dissipation from a friction model). Presto uses a kinematic approach rather than a penalty approach to eliminate the interpenetration of surfaces. In the kinematic approach, a series of constraint equations are satisfied that remove interpenetration. A penalty approach can be thought of as introducing “stiff” springs between contact surfaces as a means of preventing interpenetration.

In the current version of Presto contact between surfaces is computed as node-face interactions. To establish some key definitions for node-face contact and node-face interactions, we consider the simple two-dimensional contact problem shown in Figure 7.1. There are two blocks, \(a\) and \(b\). Block \(a\) is enclosed by surface \(a\), and block \(b\) is enclosed by surface \(b\). In finite element models, a surface is defined by a collection of finite element faces. The surface of a block of hexahedral elements, for example, is defined by a collection of quadrilateral faces on the surface of the block. For our two-dimensional example, the faces are a straight line between two nodes. We only show the faces on the portions of the surfaces that will come into contact.

Figure 7.1 shows the two blocks at time step \(n\). Figure 7.2 shows the two blocks at time step \(n + 1\). The blocks have moved and deformed under the influence of external forces. Contact has not been taken into account, and we now observe interpenetration of the two blocks. We remove this interpenetration by applying our contact algorithm.

For interpenetration to occur as shown in Figure 7.2, any node on surface \(a\) that interpenetrates surface \(b\) must pass through some face on surface \(b\). Likewise, each node on surface \(b\) that interpenetrates surface \(a\) must pass through some face on surface \(a\). We could push all the nodes on surface \(a\) so that they lie on surface \(b\), where surface \(b\) has the configuration shown in Figure 7.2.
Or we could push all the nodes on surface \( b \) so that they lie on surface \( a \), where surface \( a \) has the configuration shown in Figure 7.2. In some cases, we do use one of these two options, \( a \) to \( b \) or \( b \) to \( a \). However, we typically do something “in between” and move nodes to what can be described as an interface surface, which is shown by a thick black line in Figure 7.2. The interface surface is shown as a straight line, but it would really be a curved line in all but the most unusual cases for a two-dimensional problem like the one shown. For three-dimensional problems, the interface surface will be a complex surface in three-dimensional space.

For our “in between” solution, each node on surface \( a \) that has penetrated some face on surface \( b \), we compute some set of forces (based on the amount of node penetration) on the node on \( a \) and the nodes associated with the face on \( b \) to remove “some part” of the interpenetration. Likewise, for each node on surface \( b \) that has penetrated some face on surface \( a \), we can compute some set of forces (based on the amount of node penetration) on surface \( b \) and the nodes associated with the face on surface \( a \) to remove “another part” of the interpenetration. This node-face interaction from both contact surfaces is typically what is encountered in Presto and it is referred to as “symmetric” contact. After the nodes on both surfaces, \( a \) and \( b \), have been moved, we have defined an interface surface. A more detailed discussion of how we move the nodes on both surfaces is given in those sections related to kinematic partitioning, Section 7.14.4 and Section 7.15.2.

The simple two-dimensional example we have just discussed is analogous to much of the contact that is encountered when contact in Presto is used in an analysis. Surfaces are generated that consist of a collection of faces, each face being defined by a nodal connectivity. Node-face interactions from both contact surfaces (symmetric contact) are used to move nodes to account for any interpenetration of the surfaces. Interpenetration means we have a node on a surface that has moved through a face on an opposing surface.

Contact in Presto will handle the node-face contact just presented. It will also handle variations of the node-face contact we have just discussed. Some of these variations are as follows:
In some cases, you may want one surface of a surface pair to determine the interface surface. One surface will be designated as the master surface. The opposing surface will be designated as the slave surface. The nodes on the slave surface will be moved to the master surface. The master surface sets the interface surface. This arrangement would be a pure master-slave situation. You might want to use this arrangement if you had a very stiff surface like steel contacting a very weak surface like foam.

In some cases, you may want one surface of a surface pair to be more influential in determining the interface surface than its opposing surface. This arrangement is done by “weighting” the more influential surface and involves a concept called kinematic partitioning. The above case of pure master-slave represents the limiting case for kinematic partitioning.

A special case of contact called “tied contact” allows you to tie two surfaces on different objects together. The two surfaces that are tied together share a coincident surface or are in very close proximity at time 0.0. The initial point of contact between a tied node and an opposing face at time 0.0 is maintained for all times. At each time step, the node is moved so that it is the same point on the face regardless of where the faces move or how the face deforms.

One of the surfaces in a contact pair can be an analytic surface. An analytic surface is defined by an algebraic expression, not by a collection of faces derived from elements. The algebraic expression that defines the surface of a cylinder is an example of an analytic surface. The nodes on the opposing surface cannot penetrate the analytic surface.

Instead of having two surfaces in contact, you can have a set of nodes not associated with faces that contacts a surface. We refer to this set of nodes as a “contact node set.” The nodes in the contact node set can contact a surface that is a collection of faces (the usual surface...
CHAPTER 7. CONTACT

definition) or an analytic surface. The nodes in the contact node set cannot penetrate the surface.

- A mesh could have an initial interpenetration of two surfaces due to the meshing process. We refer to this situation as “initial overlap.” You have the option of removing this initial overlap.

- An element block can contact itself. A block of elements may deform to such an extent that a part of the surface of the block comes into contact with another part of the surface of the block. This is referred to as “self-contact.” For self-contact, a node that is part of an element block can contact a face that is exterior to the same element block.

There are some special considerations for contact with structural elements (i.e. shells, springs, trusses, beams) with the current implementation of contact. A shell element has both a top face and a bottom face that are defined by the same geometric entity. One-dimensional elements (springs, trusses, and beams) have no faces.

Shell elements are handled by the contact algorithm, but they are much more difficult to handle than solid elements. Determining whether a node has penetrated a shell element is more difficult than determining whether a node has penetrated a solid. For a solid element with an external face, there is only one normal for the face. For a shell element, there are two faces—one on each side of the geometric entity that defines the shell. Each face has a normal, and the two normals for the shell element point in opposite directions. For shell elements, two faces are constructed for the element within the contact algorithm. The faces, each with a unique outward normal, can be coincident, or they can be separated by the thickness of the shell. Separating the two shell faces that are originally coincident at the geometric plane of the shell by the thickness of the shell is referred to as “lofting.” To implement lofting, we need information about the thickness of the shell. This information is specified in the SHELL SECTION command block described in Section 5.2.2. For more information on lofting, see Section 7.9.

Contact for shell elements is only considered on shell faces; shell edges are currently not considered. The contact of a shell edge with another shell edge is not detected, and the contact of a shell edge with a continuum element edge is not detected. A shell element can coincide with the face of a continuum element. The contact algorithm will properly account for this situation. Two shell elements can also overlay each other, i.e., share the same set of nodes. The contact algorithm will also properly account for this situation. For a block of shell elements, two surfaces are created in contact.

Contact for one-dimensional elements (springs, trusses, beams) is currently implemented only for one-dimensional elements contacting a surface. The contact algorithm will not detect contact of a one-dimensional element with the edge of a continuum element, with the edge of a shell element, or with another one-dimensional element. Contact of one-dimensional elements is discussed in Section 7.2.4.

Contact in Presto is implemented in two distinct phases: a search algorithm and an enforcement algorithm. The search algorithm identifies nodes that have penetrated a face, while the enforcement algorithm computes the forces to remove penetration and the forces that observe the user-specified
surface physics. The contact search within Presto focuses on large-scale global contact in a massively parallel environment. This processing step can be quite expensive, taking upwards of 60% of the analysis time, especially on multiprocessor analyses. The search algorithm relies on normal and tangential tolerances to describe a region around each face within which any nodes found are identified as potential interactions. The size of these tolerances is problem dependent.

The enforcement algorithm is based on a kinematic approach that satisfies momentum balance by default or, optionally, a penalty approach. A kinematic approach with momentum balance enforcement, where iterations are used to ensure normal impact momentum balance and frictional response, is always more accurate than the penalty approach. Consequently, when the surface interaction involves a frictional response, the kinematic approach with momentum balance is recommended. Currently, the penalty approach is under development. Use the kinematic approach with momentum balance (the default) until the penalty approach has been fully developed and tested.

A number of friction models are available to describe the surface interactions. In this chapter on contact, we will use the term friction model for what is really a surface-physics model.

Contact within a Presto analysis is defined within a CONTACT DEFINITION command block. Within the contact definition scope, there are command lines and command blocks that define the specifics for the interaction of surfaces via the contact algorithm. Some of the command lines and command blocks within the contact scope set up default parameters that affect all contact calculations. Some of the command blocks in the contact scope affect only the interaction between a pair of surfaces.

There are three approaches that can be used to define a contact problem:

1. Accept all the Presto default parameters for a problem.
2. Accept the Presto default parameters for some of the contact surfaces. For the rest of the contact surfaces, the user can change some of the Presto default settings.
3. Define all surface-pair interactions separately.

Note that the speed of contact is based primarily on the number of nodes and faces in the contact surfaces and, to a much lesser extent, on the number of interactions specified. Consequently, choosing the third approach above is not likely to reduce the run time significantly.

The general pattern of syntax for describing contact is as follows:

- Identify all surfaces that need to be considered for contact. This is done with command lines (or command blocks) within the contact scope.

- Specify any analytic surface used for contact. Analytic surfaces are described with a command block.

- Specify any special contact options such as initial overlap removal or angle for multiple interactions. This is done with command lines within the contact scope.
- Describe friction models used in the surface interactions for this analysis. Currently, there are 11 types of friction models. Usersubroutines can also be used as friction models. A friction model is described with a command block.

- Set contact search options that will serve as defaults for all the surface interactions. These values are set in the SEARCH OPTIONS command block.

- Set contact enforcement options that will apply to all the surface interactions. These values are set in the ENFORCEMENT OPTIONS command block.

- Set default interaction values that apply to all the surface interactions. These values are set in the INTERACTION DEFAULTS command block.

- Specify values for interactions between specific contact surfaces. This is done within an INTERACTION command block. Values specified in this command block override the defaults for the particular pair of surface interactions.
7.1 Contact Definition Block

All commands for contact occur within a CONTACT DEFINITION command block. A summary of these commands follows.

BEGIN CONTACT DEFINITION <string>name
  # contact surface and node set definition
  CONTACT SURFACE <string>name
    CONTAINS <string list>surface_names
  #
  SKIN ALL BLOCKS = <string>ON|OFF(OFF)
    [EXCEPT <string list> block_names]
  #
  BEGIN CONTACT SURFACE <string>name
    BLOCK = <string list>block_names
    SURFACE = <string list>surface_names
    NODE SET = <string list>node_set_names
    REMOVE BLOCK = <string list>block_names
    REMOVE SURFACE = <string list>surface_names
    REMOVE NODE SET = <string list>nodelist_names
  END [CONTACT SURFACE <string>name]
  #
  CONTACT NODE SET <string>surface_name
    CONTAINS <string>nodelist_names
  #
  # Switch between available contact algorithms
  CONTACT FORMULATION TYPE = <string>ACME|DASH(ACME)
  # analytic surfaces
  BEGIN ANALYTIC PLANE <string>name
    NORMAL = <string>defined_direction
    POINT = <string>defined_point
  END [ANALYTIC PLANE <string>name]
  #
  BEGIN ANALYTIC CYLINDER <string>name
    CENTER = <string>defined_point
    AXIAL DIRECTION = <string>defined_axis
    RADIUS = <real>cylinder_radius
    LENGTH = <real>cylinder_length
    CONTACT NORMAL = <string>OUTSIDE|INSIDE
  END [ANALYTIC CYLINDER <string>name]
  #
  BEGIN ANALYTIC SPHERE <string>name
    CENTER = <string>defined_point
    RADIUS = <real>sphere_radius
  END [ANALYTIC SPHERE <string>name]
  # end contact surface and node set definition
UPDATE ALL SURFACES FOR ELEMENT DEATH = <string>ON|OFF(ON)

BEGIN REMOVE INITIAL OVERLAP
  OVERLAP NORMAL TOLERANCE = <real>over_norm_tol
  OVERLAP TANGENTIAL TOLERANCE = <real>over_tang_tol
  SHELL OVERLAP ITERATIONS = <integer>max_iter(10)
  SHELL OVERLAP TOLERANCE = <real>shell_over_tol(0.0)
END [REMOVE INITIAL OVERLAP]

MULTIPLE INTERACTIONS = <string>ON|OFF(ON)
MULTIPLE INTERACTIONS WITH ANGLE = <real>angle(60.0)

BEGIN SURFACE NORMAL SMOOTHING
  ANGLE = <real>angle
  DISTANCE = <real>distance
  RESOLUTION = <string>NODE|EDGE
END SURFACE NORMAL SMOOTHING

ERODED FACE TREATMENT = <string>NONE|ALL(ALL)

BEGIN SHELL LOFTING
  LOFTING ALGORITHM = <string>ON|OFF(ON)
  COINCIDENT SHELL TREATMENT = <string>DISALLOW|IGNORE|
    SIMPLE(DISALLOW)
  COINCIDENT SHELL HEX TREATMENT = <string>DISALLOW|
    IGNORE|TAPERED|EMBEDDED(DISALLOW)
END [SHELL LOFTING]

BEGIN FRICTIONLESS MODEL <string>name
END [FRICTIONLESS MODEL <string>name]

BEGIN CONSTANT FRICTION MODEL <string>name
  FRICTION COEFFICIENT = <real>coeff
END [CONSTANT FRICTION MODEL <string>name]

BEGIN TIED MODEL <string>name
END [TIED MODEL <string>name]

BEGIN SPRING WELD MODEL <string>name
  NORMAL DISPLACEMENT FUNCTION = <string>func_name
  NORMAL DISPLACEMENT SCALE FACTOR = <real>scale_factor(1.0)
TANGENTIAL DISPLACEMENT FUNCTION = <string>func_name
TANGENTIAL DISPLACEMENT SCALE FACTOR =
<real>scale_factor(1.0)
FAILURE ENVELOPE EXPONENT = <real>exponent(2.0)
FAILURE DECAY CYCLES = <integer>num_cycles(1)
FAILED MODEL = <string>failed_model_name|FRICIONLESS
(FRICIONLESS)
END [SPRING WELD MODEL <string>name]
#
BEGIN SURFACE WELD MODEL <string>name
NORMAL CAPACITY = <real>normal_cap
TANGENTIAL CAPACITY = <real>tangential_cap
FAILURE DECAY CYCLES = <integer>num_cycles(1)
FAILED MODEL = <string>failed_model_name|FRICIONLESS
(FRICIONLESS)
END [SURFACE WELD MODEL <string>name]
#
BEGIN AREA WELD MODEL <string>name
NORMAL CAPACITY = <real>normal_cap
TANGENTIAL CAPACITY = <real>tangential_cap
FAILURE DECAY CYCLES = <integer>num_cycles(1)
FAILED MODEL = <string>failed_model_name|FRICIONLESS
(FRICIONLESS)
END [AREA WELD MODEL <string>name]
#
BEGIN ADHESION MODEL <string>name
ADHESION FUNCTION = <string>func_name
ADHESION SCALE FACTOR = <real>scale_factor(1.0)
END [ADHESION MODEL <string>name]
#
BEGIN COHESIVE ZONE MODEL <string>name
TRACTION DISPLACEMENT FUNCTION = <string>func_name
TRACTION DISPLACEMENT SCALE FACTOR =
<real>scale_factor(1.0)
CRITICAL NORMAL GAP = <real>crit_norm_gap
CRITICAL TANGENTIAL GAP = <real>crit_tangential_gap
END [COHESIVE ZONE MODEL <string>name]
#
BEGIN JUNCTION MODEL <string>name
NORMAL TRACTION FUNCTION = <string>func_name
NORMAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
TANGENTIAL TRACTION FUNCTION = <string>func_name
TANGENTIAL TRACTION SCALE FACTOR =
<real>scale_factor(1.0)
NORMAL CUTOFF DISTANCE FOR TANGENTIAL TRACTION =
<real>distance
END [JUNCTION MODEL <string>name]
# BEGIN THREADED MODEL <string>name
NORMAL TRACTION FUNCTION = <string>func_name
NORMAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
TANGENTIAL TRACTION FUNCTION = <string>func_name
TANGENTIAL TRACTION SCALE FACTOR =<real>scale_factor(1.0)
TANGENTIAL TRACTION GAP FUNCTION = <string>func_name
TANGENTIAL TRACTION GAP SCALE FACTOR = <real>scale_factor(1.0)
NORMAL CAPACITY = <real>normal_cap
TANGENTIAL CAPACITY = <real>tangential_cap
FAILURE ENVELOPE EXPONENT = <real>exponent(2.0)
FAILURE DECAY CYCLES = <integer>num_cycles(1)
FAILED MODEL = <string>failed_model_name|FRICTIONLESS (FRICTIONLESS)
END [THREADED MODEL <string>name]
#
BEGIN PV_DEPENDENT MODEL <string>name
STATIC COEFFICIENT = <real>stat_coeff
DYNAMIC COEFFICIENT = <real>dyn_coeff
VELOCITY DECAY = <real>vel_decay
REFERENCE PRESSURE = <real>p_ref
OFFSET PRESSURE = <real>p_off
PRESSURE EXPONENT = <real>p_exp
END [PV_DEPENDENT MODEL <string>name]
# end surface physics models
#
BEGIN USER SUBROUTINE MODEL <string>name
INITIALIZE MODEL SUBROUTINE = <string>init_model_name
INITIALIZE TIME STEP SUBROUTINE = <string>init_ts_name
INITIALIZE NODE STATE DATA SUBROUTINE = <string>init_node_data_name
LIMIT FORCE SUBROUTINE = <string>limit_force_name
ACTIVE SUBROUTINE = <string>active_name
INTERACTION TYPE SUBROUTINE = <string>interaction_name
END [USER SUBROUTINE MODEL <string>name]
#
# search options command block
BEGIN SEARCH OPTIONS [<string>name]
GLOBAL SEARCH INCREMENT = <integer>num_steps(1)
GLOBAL SEARCH ONCE = <string>ON|OFF(OFF)
SEARCH TOLERANCE = <string>AUTOMATIC|USER_DEFINED (AUTOMATIC)
NORMAL TOLERANCE = <real>norm_tol
TANGENTIAL TOLERANCE = <real>tang_tol
SECONDARY DECOMPOSITION = <string>ON|OFF(ON)
7.1. CONTACT DEFINITION BLOCK

END [SEARCH OPTIONS <string>name]

# enforcement
BEGIN ENFORCEMENT OPTIONS [<string>name]
  ENFORCEMENT ALGORITHM = <string>MOMENTUM_BALANCE|
  PENALTY (MOMENTUM_BALANCE)
  MOMENTUM BALANCE ITERATIONS = <integer>num_iter(5)
  NUM GEOMETRY UPDATE ITERATIONS = <integer>num_iter(5)
END [ENFORCEMENT OPTIONS <string>name]

BEGIN INTERACTION DEFAULTS [<string>name]
  SURFACES = <string list>surface_names
  SELF CONTACT = <string>ON|OFF(OFF)
  GENERAL CONTACT = <string>ON|OFF(OFF)
  AUTOMATIC KINEMATIC PARTITION = <string>ON|OFF(OFF)
  INTERACTION BEHAVIOR = <string>SLIDING|
    INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)
  FRICTION MODEL = <string>friction_model_name|
    FRICTIONLESS(FRICTIONLESS)
END [INTERACTION DEFAULTS <string>name]

BEGIN INTERACTION [<string>name]
  SURFACES = <string>surface1 <string>surface2
  MASTER = <string>surface
  SLAVE = <string>surface
  KINEMATIC PARTITION = <real>kin_part
  NORMAL TOLERANCE = <real>norm_tol
  TANGENTIAL TOLERANCE = <real>tang_tol
  OVERLAP NORMAL TOLERANCE = <real>over_norm_tol
  OVERLAP TANGENTIAL TOLERANCE = <real>over_tang_tol
  FRICTION MODEL = <string>friction_model_name|
    FRICTIONLESS(FRICTIONLESS)
  AUTOMATIC KINEMATIC PARTITION
  INTERACTION BEHAVIOR = <string>SLIDING|
    INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)
END [INTERACTION <string>name]

BEGIN DASH OPTIONS
  SCALE FACTOR = <real>factor(1.0)
  DICE FACES = <string>ON|OFF (ON)
  ENFORCEMENT CONVERGENCE TOLERANCE = <real>1.0e-05
  HIDDEN SELF CONTACT = <string>TRUE|FALSE(TRUE)
END

# end enforcement
The command block begins with the input line:

```
BEGIN CONTACT DEFINITION <string>name
```

and is terminated with the input line:

```
END [CONTACT DEFINITION <string>name]
```

where name is a name for this contact definition. The name should be unique among all the contact definitions in an analysis. All other contact commands are encapsulated within this command block, as shown in the summary of the block presented previously. These other contact commands are described in Section 7.2 through Section 7.15. Section 7.16 explains how to implement contact for several example problems.

A typical analysis will have only one CONTACT DEFINITION command block. However, more than one contact definition can be used. As each CONTACT DEFINITION command block creates its own contact entity, fewer of these command blocks provide more efficient contact processing.
7.2 Descriptions of Contact Surfaces

In general, contact determines whether one surface has inter-penetrated another surface. As indicated previously, a surface is defined by an analytic representation or a collection of finite element faces. This section describes how to define a surface composed of finite element faces. It also describes how to define a set of nodes (zero-dimensional entities) not associated with faces that can contact a surface, the surface being composed of finite element faces or the surface being an analytic surface. This latter case (a node not associated with a face contacting a surface) is useful for models where, for example, we have both continuum and SPH elements. (We will refer to nodes not associated with faces as “unassociated” nodes.) Defining rigid analytic surfaces is discussed in Section 7.3.

Generally, a surface is defined as a collection of finite element faces. Both continuum elements and shell elements have faces. For a continuum element, any face that is not shared with another element can be considered for contact. For a shell element, one element can have both a top face and a bottom face. These top and bottom surfaces are automatically created for the contact algorithm and may be lofted by a user-specified thickness. Shell contact is done by computing the contact forces on the top and bottom surfaces of the shells and then moving the resulting forces back to the original shell nodes.

At this point, it is important to introduce the concept of “skinning” a block of elements. We can generate a surface (a collection of faces) from a block of continuum elements by skinning the block of elements. All exterior faces (any face not shared by two elements) will be associated with the surface for that block when the block is skinned. If we have two blocks of continuum elements that are connected (some of the element faces in one block are shared by the element faces in the other block) and we skin both of these blocks, then the skinned surface for each block will consist of faces that are exterior to both blocks. For this case, we will have generated two surfaces. The set of external faces from skinning the first block will have a unique surface name, and the set of external faces generated by skinning the second block will have a unique surface name. Any face shared by the two blocks will not be in the surfaces derived by skinning the two blocks. If we have a single block of shell elements and we skin the block, then all the top faces of all the shell elements will be one surface and the bottom faces of all the shell elements will be another surface. (In Presto we do not have to be concerned with naming two distinct surfaces for shell elements. This is handled internally by the code.) Suppose we have two blocks of shell elements in which none of the elements in one block overlap the elements in another block; the two blocks are joined only at the shell edges. In this case, we will get a unique surface identifier that references both the top and bottom faces of all the shell elements in the first block, and we will get a unique surface identifier that references both the top and bottom faces of all the shell elements in the second block.

Skinning becomes more complicated when we have a shell surface that overlays the surface of a block of continuum elements. If a shell surface overlays the surface of a block of continuum elements, we can have shell elements that are coincident with the external faces of the continuum elements. Coincident in this case means that a shell element has the same nodal connectivity as the nodal connectivity defining an external face of a continuum element. Skinning also becomes more complicated when we have two shell blocks with coincident elements. Coincident in this case means we have two shell elements in different blocks that have the same nodal connectivity.
See Section 7.9 for more information about skinning with shells.

A face can only be associated with a single contact surface. However, in the process of defining contact surfaces, you might create a situation where one face appears on more than one contact surface. If a face appears on more than one contact surface, an ambiguous situation arises. The following example should help to explain this ambiguous situation.

First, let us establish a situation where there is a face that appears on two contact surfaces. One contact surface is defined by skinning an element block of hexahedral elements. The name of this surface obtained by skinning a block is block_1024. One of the faces in surface block_1024 is defined by the node connectivity \{100, 101, 1002, 1001\}. A surface on the same element block is defined by specifying a side set definition. The name of this surface obtained by using a side set definition is surface_1000. One of the faces in surface surface_1000 is defined by the node connectivity \{100, 101, 1002, 1001\}. In this example, we have the same face, \{100, 101, 1002, 1001\}, defined on two different surfaces, block_1024 and surface_1000. The definition of the surface with the side set includes one of the faces in the surface obtained by skinning the block.

Now let us show how an ambiguous situation can arise. Suppose, in our example, that the friction model specified for surface block_1024 is different from the friction model specified for surface surface_1000. Furthermore, suppose that the tolerances specified for surface block_1024 are different from the tolerances specified for surface surface_1000. For contact, only one friction model and only one set of tolerances can be applied to face \{100, 101, 1002, 1001\}. The question arises as to which friction model and which set of tolerances should be applied to the face. Any face, in general, can have only one type of a given contact property—friction model, tolerances, etc.—applied to the face.

To handle the case of a face defined in more than one contact surface, any face defined in more than one contact surface will be assigned to the first contact surface defined in the CONTACT DEFINITION command block that includes the face. For example, if contact surface block_1024 is defined before contact surface surface_1000 in the CONTACT DEFINITION command block, then face \{100, 101, 1002, 1001\} will be assigned to contact surface block_1024. Face \{100, 101, 1002, 1001\} will not be assigned to contact surface surface_1000. In general, then, any face appearing on multiple contact surfaces will be assigned to the first contact surface defined in the CONTACT DEFINITION command block that includes the face. (The ordering of the contact surface definitions in the CONTACT DEFINITION command block will determine how faces defined on multiple contact surfaces are assigned to a contact surface.) If a face is defined on multiple contact surfaces, a warning is generated.

For the case where unassociated nodes are contacting a surface, you will need to define some collection of unassociated nodes and a surface that can be contacted by these nodes. SPH particles contacting a surface is an example of nodes contacting a surface. The contact of one-dimensional elements (springs, trusses, beams) with a surface can also be modeled as unassociated nodes contacting a surface, although, as in the case of shells, there are some limitations. The contact algorithm cannot detect a one-dimensional element cutting through the edge of a shell element, the edge of a continuum element, or through another one-dimensional element.

To describe surfaces defined by finite element faces that can be considered for contact, you can use the CONTACT SURFACE command line, the SKIN ALL BLOCKS command line, or the CONTACT
SURFACE command block. To describe unassociated nodes that can come into contact with surfaces, you should use the CONTACT NODE SET command line or the CONTACT SURFACE command block. A CONTACT DEFINITION command block can contain any combination of these command lines and command blocks provided that no two of these commands have the same name. The CONTACT DEFINITION command block MUST include some type of surface definition. Any element faces or unassociated nodes that you want to use for contact interaction must be identified as contact faces or contact nodes, respectively.

Section 7.2.1 through Section 7.2.4 describe the command lines and command blocks for defining contact surfaces composed of finite element faces and node sets that can contact surfaces.

7.2.1 Contact Surface Command Line

CONTACT SURFACE <string>name
CONTAINS <string list>surface_names

This command line identifies a set of surfaces (specified as side sets) and element blocks that will be considered as a single contact surface; the string name is the unique name for this contact surface. The list denoted by surfaces_names is a list of strings identifying surfaces that are to be associated with this contact surface name. The surfaces can be side sets, element blocks, or any combination of the two as defined in the exodus file. These are not names of analytic surfaces. Any specified element blocks are “skinned,” i.e., a surface is created from the exterior of the element block. See the previous discussion on skinning. Blocks of shell elements will be skinned, and the shell surfaces generated from a CONTACT SURFACE command line will be lofted for contact if the lofting algorithm is ON in the SHELL LOFTING command block.

If a block of one-dimensional elements (springs, trusses, beams) is included in the list of surface_names, the element block will be ignored. Thus, to include the one-dimensional elements for contact, a CONTACT NODE SET command line should be used. See Section 7.2.4.

The name you create for a surface can be referenced in command blocks that specify how that surface will interact with another contact surface or with itself. See Section 7.14.1 and Section 7.15.1.

The surfaces can contain a heterogeneous set of face types as well as any number of side sets and element blocks.

If a face appears in a side set and also in a set of faces generated by the skinning of an element block, that face will produce an error. As indicated previously, any given face may not appear in more than one contact surface.

7.2.2 Skin All Blocks

SKIN ALL BLOCKS = <string>ON|OFF(OFF)
[EXCEPT <string list>block_names]

You may wish to consider contact between the external surfaces of all the element blocks in the mesh. The SKIN ALL BLOCKS command line causes all element blocks to be “skinned,” i.e.,
a surface is created from the exterior of each element block. The skinned surfaces are then given contact surface names identical to the name of the element block. For instance, if a mesh contained the element blocks block_1, block_10, and block_11, then SKIN ALL BLOCKS would create three contact surfaces from these blocks with the names block_1, block_10, and block_11, respectively.

You can selectively delete some blocks from skinning by using the EXCEPT option. Any blocks you do not want to be skinned will be included in a list of block names following EXCEPT.

The SKIN ALL BLOCKS is useful for large models in which the individual specification of contact surfaces would be unwieldy.

If the SKIN ALL BLOCKS command line is used without the EXCEPT option, contact surfaces cannot be defined by the above CONTACT SURFACE command line or the CONTACT SURFACE command block. The use of the SKIN ALL BLOCKS command line without the EXCEPT option would include all exterior faces for all element blocks in the set of contact surfaces generated by the SKIN ALL BLOCKS command line. The added use of a CONTACT SURFACE command line or CONTACT SURFACE command block would then generate a new surface that would have to include at least one exterior face. But all exterior faces have been included in the surfaces generated by the SKIN ALL BLOCKS command line (without the EXCEPT option). This creates a situation where we have the same face in two different surfaces. Specifying the same face in two different contact surfaces is not allowed. See the example discussed in the introductory part of Section 7.2.

If you use the EXCEPT option, you can use a CONTACT SURFACE command line or the CONTACT SURFACE command block as long as you do not reference the same face on different surfaces when defining the various contact surfaces.

The CONTACT SURFACE command block, if it is used to defined a set of unassociated nodes for a contact node set, and the CONTACT NODE SET command line can be used with the SKIN ALL BLOCKS command line regardless of whether or not it uses the EXCEPT option.

If the mesh includes blocks of shell elements, the shell surfaces generated from a SKIN ALL BLOCKS command line will be lofted for contact according to the lofting algorithm specified in the SHELL LOFTING command block.

If the mesh includes blocks of one-dimensional elements (beams, trusses), the element blocks with one-dimensional elements are ignored in contact. Thus, to include the one-dimensional elements for contact, a CONTACT NODE SET command line should be used. See Section 7.2.4.

7.2.3 Contact Surface Command Block

BEGIN CONTACT SURFACE <string>name
    BLOCK = <string list>block_names
    SURFACE = <string list>surface_names
    NODE SET = <string list>node_set_names
    REMOVE BLOCK = <string list>block_names
    REMOVE SURFACE = <string list>surface_names
    REMOVE NODE SET = <string list>node_set_names
END [CONTACT SURFACE <string>name]
The **CONTACT SURFACE** command block can be used to define a contact surface consisting of a collection of finite element faces or a set of unassociated nodes that will be a contact node set. We can use some combinations of the above command lines as a set of Boolean operations to define our collection of faces or collection of unassociated nodes. The result of this command block must be either a set of faces or a set of nodes.

If you want to define a surface named `name` that is a set of faces, you can use some combination of the command lines **BLOCK**, **SURFACE**, **REMOVE BLOCK**, and **REMOVE SURFACE**. For this case, however, the **BLOCK** and **REMOVE BLOCK** command lines must refer to element blocks that are continuum or shell elements. If the element block referred to is a block of continuum elements, the block is skinned. If the element block referred to is a block of shell elements, the top and bottom faces of the shell elements will form the contact faces.

Suppose you specify a **BLOCK** command line that references several continuum blocks. The set of faces defining the surface will consist of the exterior faces for all the element blocks. If you want to preserve the list of element blocks on the **BLOCK** command line while removing the exterior faces associated with one or more of the blocks, you could simply add a **REMOVE BLOCK** command line listing only those blocks whose associated faces are to be removed from the contact surface.

**Example:**

```plaintext```
```
Suppose you specify a **BLOCK** command line that references a block of continuum elements and a **SURFACE** command line that references a side set. Then the contact surface produced by the command block will be the union of the faces defined by the skinning of the block of continuum elements and the faces defined in the side set.

Suppose you specify a **BLOCK** command line that references a block of continuum elements and a **REMOVE SURFACE** command line that references a side set. Furthermore, suppose that the side set is a set of faces that is a subset of the set of faces obtained from skinning the continuum block. Then the contact surface produced by the command block will be the set of faces obtained by skinning the continuum block minus the faces in the side set.

As can be seen from the above examples, we can use the command lines **BLOCK**, **SURFACE**, **REMOVE BLOCK**, and **REMOVE SURFACE** as Boolean operators to construct a set of finite element faces defining a surface. The **BLOCK** and **REMOVE BLOCK** command lines should produce (or remove) faces, however, so that we are performing the Boolean operations on like topological entities. See Section 7.2.4 for further information about using a node set that contacts a surface.

If you want to define a set of unassociated nodes for contact with a surface, you can use some combination of the command lines **BLOCK**, **NODE SET**, **REMOVE BLOCK**, and **REMOVE NODE SET**. For this case, however, the **BLOCK** and **REMOVE BLOCK** command lines must refer to element blocks that are SPH elements, which are topologically equivalent to a node.

**Example:**

```plaintext```
```
Suppose you specify a **BLOCK** command line that references a block of SPH elements and a **NODE SET** command line that references a node set within a command block. Then the node set produced by the command block will be the union of the nodes defined by the SPH elements and the nodes defined in the node set.

Suppose you specify a **BLOCK** command line that references a block of SPH elements and a **REMOVE NODE SET** command line that references a node set. Furthermore, suppose that the node set is a set of nodes that is a subset of the set of nodes in the SPH block. Then the set of nodes produced
by the command block will be the set of nodes obtained from the SPH block minus the nodes in the node set.

There must be at least one BLOCK, SURFACE, or NODE SET command line in the command block.

### 7.2.4 Contact Node Set

```
CONTACT NODE SET <string>surface_name
    CONTAINS <string list>nodelist_names
```

As indicated previously, contact interactions may also be defined between a surface and a set of nodes. The `CONTACT NODE SET` command line names a set of nodes (the parameter `surface_name` in the above command line) as a collection of nodes in various node sets specified by the `string list nodelist_names`. All the nodes in the node set can then interact with a contact surface. If a node in the node set defined as `surface_name` attempts to penetrate a contact surface, the node will be moved to the surface through the contact calculations.

The node defined by the `CONTACT NODE SET` command line will be paired with either a mesh surface or an analytic surface when contact interactions are defined. In defining interactions between a contact node set and another surface, the interaction must be defined as a pure master-slave interaction, where the nodes in the contact node set are the slave nodes. The master-slave interaction is defined in the `INTERACTION` command block (see Section 7.15). The easiest way to define the correct relation between the nodes in the node set and the faces in the actual surface is to pair the surface with the `MASTER` command line and the node set with the `SLAVE` command line. Suppose the set of nodes is named `beam_nodes` on the `CONTACT NODE SET` command line and the surface these nodes are paired with is named `plate`. Then the `INTERACTION` command block for the interaction of the node set and surface would contain the command lines below.

```
MASTER = plate
SLAVE = beam_nodes
```

Presto will not detect whether or not you have specified a master-slave relation between a surface and a set of nodes. If the interaction between a surface and a set of nodes defaults to a kinematic partition value of 0.5 and there is only one enforcement iteration, then any nodes that have penetrated the surface will only be moved one-half the penetration distance. Therefore, you should check your input carefully if you have an interaction between a surface and a node set to make sure that the master-slave relation has been properly defined for this interaction.

The `CONTACT NODE SET` command line is used to define contact interactions between SPH particles and other contact surfaces—faces on solid elements, shell/membrane faces, and analytic surfaces. The `CONTACT NODE SET` command line also presents a simple approach for contact between one-dimensional elements (beams, trusses) and other contact surfaces—faces on solid elements, shell/membrane faces, and analytic surfaces. In this case, contact processing will seek to remove interpenetration of the nodes of the one-dimensional elements into the other contact surfaces. The contact capabilities in Presto will not currently handle any contact between two one-dimensional elements.
7.3 Analytic Contact Surfaces

Presto permits the definition of rigid analytic surfaces for use in contact. Contact evaluation between a deformable body and a rigid analytic surface is much faster than contact evaluation between two deformable bodies. Therefore, using a rigid analytic surface is more efficient than using a very stiff deformable body to try to approximate a rigid surface. The commands for defining the rigid analytic surfaces currently available in Presto—plane, cylinder, and sphere—are described next.

7.3.1 Plane

```
BEGIN ANALYTIC PLANE <string>name
  NORMAL = <string>defined_direction
  POINT = <string>defined_point
END [ANALYTIC PLANE <string>name]
```

Analytic planes are not deformable, they cannot be moved, and two analytic planes will not interact with each other. The `ANALYTIC PLANE` command block for defining an analytic plane begins with the input line:

```
BEGIN ANALYTIC PLANE <string>name
```

and is terminated with the input line:

```
END [ANALYTIC PLANE <string>name]
```

where the string `name` is some user-selected name for this particular plane. This name is used to identify the surface in the interaction definitions. The string `defined_direction` in the `NORMAL` command line refers to a vector that has been defined with a `DEFINE DIRECTION` command line; this vector defines the outward normal to the plane. The string `defined_point` in the `POINT` command line refers to a point in a plane that has been defined with a `DEFINE POINT` command line. The deformable body should initially be on the side of the plane defined by the outward normal.

7.3.2 Cylinder

```
BEGIN ANALYTIC CYLINDER <string>name
  CENTER = <string>defined_point
  AXIAL DIRECTION = <string>defined_axis
  RADIUS = <real>cylinder_radius
  LENGTH = <real>cylinder_length
  CONTACT NORMAL = <string>OUTSIDE|INSIDE
END [ANALYTIC CYLINDER <string>name]
```

Analytic cylindrical surfaces are not deformable, they cannot be moved, and two analytic cylindrical surfaces will not interact with each other. The `ANALYTIC CYLINDER` command block for
defining an analytic cylindrical surface begins with the command line:

```
BEGIN ANALYTIC CYLINDER <string>name
```

and is terminated with the command line:

```
END [ANALYTIC CYLINDER <string>name]
```

where the string **name** is some user-selected name for this particular cylindrical surface. This name is used to identify the surface in the interaction definitions. The cylindrical surface has a finite length; the cylindrical surface is not an infinitely long surface. To fully specify the location of the cylindrical surface, therefore, you must specify the center point of the cylindrical surface in addition to the axial direction of the cylinder. These quantities, center point and direction, are defined by the `CENTER` and `AXIAL DIRECTION` command lines, respectively. The string `defined_point` in the `CENTER` command line refers to a point that has been defined with a `DEFINE POINT` command line; the string `defined_axis` in the `AXIAL DIRECTION` command line refers to a vector that has been defined with a `DEFINE DIRECTION` command line. The radius of the cylinder is the real value `cylinder_radius` specified with the `RADIUS` command line, and the length of the cylinder is the real value `cylinder_length` specified by the `LENGTH` command line. The length of the cylinder (`cylinder_length`) extends a distance of `cylinder_length` divided by 2 along the cylinder axis in both directions from the center point. If the rigid surface is the outside of the cylinder, you should specify:

`CONTACT NORMAL = OUTSIDE`

If the rigid surface is the inside of the cylinder, you should specify:

`CONTACT NORMAL = INSIDE`

### 7.3.3 Sphere

```
BEGIN ANALYTIC SPHERE <string>name
   CENTER = <string>defined_point
   RADIUS = <real>sphere_radius
END [ANALYTIC SPHERE <string>name]
```

Analytic spherical surfaces are not deformable, they cannot be moved, and two analytic spherical surfaces will not interact with each other. The `ANALYTIC SPHERE` command block for defining an analytic spherical surface begins with the input line:

```
BEGIN ANALYTIC SPHERE <string>name
```

and is terminated with the input line:

```
END [ANALYTIC SPHERE <string>name]
```

where the string **name** is some user-selected name for this particular spherical surface. This name is used to identify the surface in the interaction definitions. The center point of the sphere is defined by the `CENTER` command line, which references a point, `defined_point`, specified by a `DEFINE POINT` command line. The radius of the sphere is the real value `sphere_radius` specified with the `RADIUS` command line.
7.4 Update All Surfaces for Element Death

\[ \text{UPDATE ALL SURFACES FOR ELEMENT DEATH} \]
\[ = \text{<string>ON|OFF(ON)} \]

When elements are killed in an analysis, contact surfaces may need to be updated to account for the removal of faces attached to killed elements or the addition of faces exposed by element death. The command line UPDATE ALL SURFACES FOR ELEMENT DEATH permits contact surfaces to be updated based on all the ELEMENT DEATH command block(s) specified in the input file (see Section 5.5). This update of contact surfaces is controlled by the command line being set to ON, the default. The update encompasses the full reinitialization of contact. Thus, surface-physics models that involve state data may lose some information when the new contact surfaces are created. If the command line is set to OFF, an element associated with a face on the contact surface could be killed, but the face would remain in the list of faces defining the contact surface, which may be unacceptable for your analysis.
7.5 Remove Initial Overlap

BEGIN REMOVE INITIAL OVERLAP
OVERLAP NORMAL TOLERANCE = <real>over_norm_tol
OVERLAP TANGENTIAL TOLERANCE = <real>over_tang_tol
SHELL OVERLAP ITERATIONS = <integer>max_iter(10)
SHELL OVERLAP TOLERANCE = <real>shell_over_tol(0.0)
END REMOVE INITIAL OVERLAP

Meshes supplied for finite element analyses frequently have some level of initial mesh overlap, where finite element nodes rest inside the volume of elements. This can cause problems with contact; overlaps may cause initial forces that are nonphysical and produce erroneous stress waves. Presto provides a mechanism to modify the initial mesh to attempt to remove overlaps in surfaces defined for contact via the REMOVE INITIAL OVERLAP command block.

The process used to remove the initial overlap for three-dimensional solid elements involves changing the original coordinates of nodes on contact surfaces. Changing the coordinates yields a new mesh with the overlap removed; the overlap removal adds no initial stresses. Normal and tangential tolerances are specified by the user for all the contact surfaces in the REMOVE INITIAL OVERLAP command block. It is also possible to specify overlap normal and tangential tolerances on each surface pairing separately in the INTERACTION command block. In other words, overlap removal tolerances specified in INTERACTION command blocks will overwrite the tolerances specified in the REMOVE INITIAL OVERLAP command block. See Section 7.15 for details. The REMOVE INITIAL OVERLAP command block only removes overlaps that are detected along the surfaces defined for contact and not all surfaces in the mesh.

Overlap tolerances are used to designate a box around each surface pair to search for overlaps. If the overlap of the mesh is larger than the box defined by the tolerances, then the overlap will not be found and thus will not be removed. However, if the specified tolerances are larger than an element length in the analysis, the overlap removal mechanism may invert elements, leading to analysis failure. This has two ramifications. First, the tolerances must be carefully specified to correct mesh overlaps and to not invert elements. Second, this mechanism is unable to remove initial overlaps that are greater than an element length. In such cases, the overlap must be removed manually using a meshing tool. The mesh modification done by the REMOVE INITIAL OVERLAP feature changes the meshed geometry, and thus can change the mass and time step of affected elements. The mesh returned in the results file includes the changed coordinates and should be checked to ensure that the modifications are acceptable. A summary of the overlap that is removed is reported in the log file. (See Section 1.7 for a discussion of the log file.) The log file lists each block in which the initial overlap has been removed as well as the maximum amount of overlap for each of these blocks. Additionally, you can request that a nodal variable called REMOVED_OVERLAP be written to the results file. See Section 8.1.1.1 for a discussion of the output of nodal variables to the results file.

For contact between shell elements, a slightly different approach is used. Because the thickness of a shell must be preserved when shell lofting is requested, removing the initial overlap between nested shells becomes an iterative process whereby shell locations are adjusted to remove the overlap. This process is approximate and may not remove all the overlap in all cases. It is advised
to check the corrected mesh to make sure that the mesh modifications are acceptable. In the input, two additional input lines, SHELL OVERLAP ITERATIONS and SHELL OVERLAP TOLERANCE, may be needed to properly remove the initial overlap.

- The SHELL OVERLAP ITERATIONS command line controls the maximum number of iterations that will be used by the overlap removal mechanism to resolve nested shells. By default, the value of max_iter is 10. If the mesh has only a few layers of shells that may overlap, a value of 10 should suffice. However, if the mesh has a number of layers of shells that may overlap, this value may need to be much larger.

- The SHELL OVERLAP TOLERANCE command line specifies an amount of overlap, shell_over_tol, that is permitted to be left in the shell elements. This helps to limit the actual number of iterations required to remove the shell overlap, and to spread any remaining overlap over a number of shells instead of concentrating it all in a single shell. If the default value of 0.0 for the shell overlap tolerance is used, iteration continues until either all the overlap is removed or the maximum number of iterations is reached. If a nonzero value for the shell overlap tolerance is used, iteration continues until the tolerance is reached or the maximum number of iterations is reached. Note that the overlap removal process is only done once during an analysis, so a large number of iterations will only affect the first time step, not every time step.

The SHELL OVERLAP ITERATIONS and SHELL OVERLAP TOLERANCE commands have no meaning for analyses that do not have shell elements.
7.6 Angle for Multiple Interactions

MULTIPLE INTERACTIONS = <string>ON|OFF(ON)
MULTIPLE INTERACTIONS WITH ANGLE = <real>angle(60.0)

When a node lies on the edge of a body, that node may need to support contact interactions with more than one face at the same time. For instance, see Figure 7.3. In Figure 7.3a, three blocks are shown, with a single node identified. Through contact, this node can interact with both the block on the upper right and the block on the bottom. If the node only supports a single interaction, then it will be arbitrarily considered for contact between one of the blocks, but not the other, as in Figure 7.3b. In this case, contact enforcement will prevent penetration into the lower block, but may permit penetration into the upper right block. The proper way to deal with this case is shown in Figure 7.3c, where multiple interactions are considered at the node.

![Figure 7.3: Illustrations of multiple interactions at a node: (a) initial configuration, with node of interest identified; (b) single interaction; and (c) multiple interactions.](image)

By default, Presto permits multiple interactions at a node. However, these multiple interactions may incur extra cost in the contact algorithm by increasing the number of interactions in enforcement. Also, a local search algorithm (see Section 7.12), which uses various contact tracking approaches, may operate more efficiently when the node can only have one interaction. Finally, multiple interactions may lead to instabilities that can be eliminated by switching to single interactions. For these reasons, the MULTIPLE INTERACTIONS command line allows the user to choose whether multiple interactions should be considered at a node. A value of OFF indicates that a node can have only one interaction. This value affects all interactions in a contact definition. Presto does not currently have the capability to force single interactions for some surface pairs while allowing multiple interactions for other surface pairs.

When the MULTIPLE INTERACTIONS command line is ON, the number of interactions that can be considered at a node is dependent on the measure of curvature of those faces that are connected to the node. If the angle between two faces on which the node is attached is small, then only one interaction is allowed. However, in cases where the angle between the faces is large enough such that they form a discrete corner, multiple interactions are considered. The contact algorithms can...
properly handle only a limited number of interactions per node (currently three), so it is generally feasible to properly define interactions at a node, e.g., at the corner of a block.

The critical angle for multiple interactions is set with the `MULTIPLE INTERACTIONS WITH ANGLE` command line, where `angle` is the angle over which an edge is considered sharp. If the angle between adjoining faces is greater than this critical angle, multiple interactions can be created. By default, this critical angle is 60 degrees, which works well for most analyses. This value can be changed in the contact input if needed.
7.7 Surface Normal Smoothing

BEGIN SURFACE NORMAL SMOOTHING
  ANGLE = <real>angle(60.0)
  DISTANCE = <real>distance(0.01)
  RESOLUTION = <string>NODE|EDGE(NODE)
END SURFACE NORMAL SMOOTHING

Surface normal smoothing is a feature that is primarily used in Adagio.

Finite element discretization often results in models with faceted edges, while the true geometry of the part is actually smoothly curved. If the faces of adjacent finite elements on a surface have differing normals, the discontinuities at the edges between those faces can cause problems with contact. These discontinuities in the face normals are particularly troublesome with an implicit code such as Adagio, which uses an iterative solver to obtain a converged solution at every step. If a node is in contact near an edge with a normal discontinuity, the node may slide back and forth between the two neighboring faces during the iterations. Because the normal directions of the two faces differ, this can make it difficult to converge on a solution to this discontinuous contact problem.

Surface normal smoothing is a technique that creates a smooth variation in the normal near edges. The normal varies linearly from the value on one face to the value on the other face over a distance that spans the edge. A smoothly varying normal at the edge makes it much easier for an iterative solver to obtain a converged solution in the case where a node has penetrated near the edge of a face.

Presto does not use an iterative solver and thus does not encounter the difficulties associated with face normal discontinuities. Consequently, the SURFACE NORMAL SMOOTHING command block is not typically useful for Presto models. It is provided in both Presto and Adagio, however, to provide a consistent transition between the two codes if they are used together in a coupled analysis.

If the SURFACE NORMAL SMOOTHING command block is present, this feature is activated. There are three optional commands that can be used within this block to control the behavior of normal smoothing.

- The ANGLE command is used to control whether smoothing should occur between neighboring faces. If the angle between two faces is less than the specified angle (given in degrees), smoothing is activated between them. Otherwise, the discontinuity is considered to be a feature of the model rather than an artifact of meshing, and they are not smoothed. The default value for angle is 60.

- The DISTANCE command specifies the distance as a fraction of the face size over which smoothing should occur. The specified value can vary from 0 to 1. The default value for distance is 0.01.

- The RESOLUTION command specifies the method used to determine the smoothed normal direction. The default NODE option uses a node-based algorithm to fit a smooth curve, while the EDGE option uses an edge-based algorithm.
7.8 Eroded Face Treatment

\[ \text{ERODED FACE TREATMENT} = \langle \text{string}\rangle \text{ALL|NONE(ALL)} \]

The ERODED FACE TREATMENT command line is used to define what happens to newly exposed element faces when a contact surface erodes because of element death. This command line applies to the case in which a contact surface has been generated by the skinning of an element block (Section 7.2). Suppose we have a contact block that has been skinned to create a contact surface, and let us consider an element that contributes a face to the original contact surface. If this element is killed at some point by element death, the death of this element exposes new faces. If the \text{ALL} option in the command line has been selected, any newly exposed faces will be included in the updated contact definition. If the \text{NONE} option is used, the faces exposed by element death will not be included in the updated contact surface. Both options will remove any faces on killed elements from the contact definition, though the \text{NONE} option tends to be more robust on complex geometries, such as those containing equivalenced elements, shell elements sandwiched between solid elements, and degenerate elements.

The default option is \text{ALL}.
7.9 Shell Lofting

BEGIN SHELL LOFTING  
LOFTING ALGORITHM = <string>ON|OFF(ON)
COINCIDENT SHELL TREATMENT = <string>DISALLOW|IGNORE|
SIMPLE(DISALLOW)
COINCIDENT SHELL HEX TREATMENT = <string>DISALLOW|
IGNORE|TAPERED|EMBEDDED(DISALLOW)
END [SHELL LOFTING]

Presto can also assess contact on shell elements. Shell elements can interact with other shell elements, faces of solid elements, and contact node sets (such as SPH). Contact on shell elements can occur on either the meshed shell geometry, i.e., ignoring any shell thickness, or on the “lofted” geometry, i.e., a geometry that includes the thickness of the shell. Currently, contact appears to be more robust on the non-lofted geometry; however, for simulations in which the thickness is important, the lofted geometry can provide more-reasonable results. Also critical to shell contact is how shells that are fully coincident with other elements (i.e., share all their nodes with another element) are treated. These options are controlled by the user in the SHELL LOFTING command block.

The LOFTING ALGORITHM command line determines whether contact on a shell should be done on the lofted geometry or on the original shell geometry. If the value of the LOFTING ALGORITHM command line is set to ON, shell contact uses the lofted geometry; if it set to OFF, shell contact uses the original shell geometry.

The COINCIDENT SHELL TREATMENT command line identifies how shells that share the same nodes should be treated. If the DISALLOW option is selected, (the default), then any time that shells in contact are detected to share all the same nodes, the code will abort with an error message indicating which elements were found to be coincident. The DISALLOW option should be used if you do not want any coincident shells to be considered in the analysis. The option operates essentially as a check on the mesh. If the IGNORE option is selected, any contact faces attached to coincident shells are ignored for contact. This option is only provided as a backup approach if undiagnosed code problems arise from coincident shells. If such a case occurs, the IGNORE option may permit the user to continue with an analysis while the code team diagnoses the problem. The SIMPLE option enables coincident shells to be processed correctly. If lofting has been enabled and the SIMPLE option is selected, the thickness of the lofted coincident shell is taken as the largest thickness of all the coincident shells. If lofting is off and the SIMPLE option is selected, the coincident shell is treated as if only one of the shells is present.

The COINCIDENT SHELL HEX TREATMENT command line has a function similar to that of the COINCIDENT SHELL TREATMENT command line. The COINCIDENT SHELL HEX TREATMENT command line, however, identifies how shells that are fully coincident with the hex elements are treated. If the DISALLOW option is selected (the default), then any time that a shell in contact is detected to share all the same nodes with the face of a continuum element, the code will abort with an error message indicating which elements were found to be coincident. The DISALLOW option should be used if you do not want any shells coincident with hexes to be considered in the analysis. The option operates essentially as a check on the mesh. If the IGNORE option is
selected, any contact faces attached to shells that are coincident with faces of continuum elements are ignored for contact. This option is only provided as a backup approach if undiagnosed code problems arise from coincident shells and continuum elements. If such a case occurs, the \texttt{IGNORE} option may permit the user to continue with an analysis while the code team diagnoses the problem. The \texttt{TAPERED} and \texttt{EMBEDDED} options permit shells that are coincident with faces of continuum elements to be processed in contact. The \texttt{TAPERED} option does two things: it includes for contact any faces that are on the free surface and ignores faces sandwiched between the shell and the continuum element, and it automatically adjusts the lofting of the surfaces to provide a smooth transition between shells that are not coincident with the faces of the continuum elements and those that are coincident with the faces of the continuum elements. The \texttt{EMBEDDED} option includes for contact both free surface faces and those that are between the coincident shells and faces of the continuum elements; the option does not adjust thicknesses to make smooth transitions between shells that are not coincident with faces of continuum elements and those that are coincident with faces of continuum elements. In general, the \texttt{TAPERED} option is preferred; only use the \texttt{EMBEDDED} option if the \texttt{TAPERED} option causes a code problem.
7.10 Contact Output Variables

To provide more information about the enforcement of contact interactions, Presto can provide additional contact variables for output. Currently, information on only one interaction at each node is provided. If a node has more than one interaction, the last one in its internal interaction list is reported.

The additional nodal contact variables that can be output are listed in Table 7.1. The variables can be output in history files or results files; see Chapter 8 for more information on outputting nodal variables. Note that currently the variables cannot be calculated at output time so the first time they are output a request is made to calculate them. This means that the first output step where they are to appear the data will be all zero. A work around for this is to have at least one output step in which these variables appear before their values are needed.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>contact_status</td>
<td>Status of the interactions at the node. Possible values are as follows: 0.0 = Node is not a contact node (not in a defined contact surface) 0.5 = Node is not in contact 1, 2, or 3 = Node has 1, 2, or 3 interactions</td>
</tr>
<tr>
<td>contact_normal_direction</td>
<td>Vector direction of the constraint. This is, in general, the normal of the face in the interaction.</td>
</tr>
<tr>
<td>contact_tangential_direction</td>
<td>Velocity of the node relative to the face times the time step minus the component of this vector along the normal to the face. Note that this vector is NOT normalized.</td>
</tr>
<tr>
<td>contact_normal_force_magnitude</td>
<td>Magnitude of the contact force at the node in the direction normal to the contact face (contact_normal_direction).</td>
</tr>
<tr>
<td>contact_tangential_force_magnitude</td>
<td>Magnitude of the contact force at the node in the plane of the contact face (contact_tangential_direction).</td>
</tr>
</tbody>
</table>

Continued on next page
7.10. CONTACT OUTPUT VARIABLES

Table 7.1 – Continued from previous page

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>contact_normal_traction_magnitude</td>
<td>Traction normal to the contact face, i.e., contact_normal_force_magnitude scaled by contact_area. If there are multiple interactions for this node, the traction only for the last interaction is given.</td>
</tr>
<tr>
<td>contact_tangential_traction_magnitude</td>
<td>Traction in the plane of the contact face, i.e., contact_traction_force_magnitude scaled by contact_area. If there are multiple interactions for this node, the traction only for the last interaction is given.</td>
</tr>
<tr>
<td>contact_slip_increment_current</td>
<td>Increment of slip tangential to the face that occurs over the time step.</td>
</tr>
<tr>
<td>contact_frictional_energy_dissipation</td>
<td>Amount of frictional energy dissipated over the time step.</td>
</tr>
<tr>
<td>contact_area</td>
<td>Contact area for the node. This is the tributary area around the node for this interaction. If there are multiple interactions, the reported area is the area associated with the last interaction.</td>
</tr>
<tr>
<td>contact_current_gap</td>
<td>Value of the gap for the current time step. If the node has multiple interactions, the reported gap is for the last interaction.</td>
</tr>
<tr>
<td>contact_previous_gap</td>
<td>Value of the gap for the previous time step. If the node has multiple interactions, the reported gap is for the last interaction.</td>
</tr>
</tbody>
</table>
7.11 Friction Models

To describe the physics of interactions that occur between contact surfaces, the Presto input for contact relies upon the definition of friction models. The user then relates these friction models to pairs of interactions in the interaction-definition blocks (see Section 7.14 and Section 7.15). During the search phase of contact, node-face interactions are identified, and the designated friction model is used to determine how the resulting contact forces are resolved between these pairs.

Currently, there are 11 primary friction models: frictionless contact, constant coulomb friction, tied contact, spring weld, surface weld, area weld, adhesion, cohesive zone, junction, threaded joint, and pressure-velocity–dependent friction. In addition, models defined by user subroutines can be used as friction models. By default, interactions between contact surfaces that have not had friction models assigned are treated as frictionless. All friction models are command blocks, although some of the models do not have any command lines inside the command block. The commands for defining the available friction models are described next. Friction models are associated with specific pairings of contact surfaces through the interaction-definition blocks in Section 7.14 and Section 7.15. Presto uses the ACME library for contact enforcement. See the documentation for ACME to obtain a more in-depth description of the implementation and usage for the various friction models.

7.11.1 Frictionless Model

```
BEGIN FRICTIONLESS MODEL <string>name
END [FRICTIONLESS MODEL <string>name]
```

The FRICTIONLESS MODEL command block defines frictionless contact between surfaces. In frictionless contact, contact forces are computed normal to the contact surfaces to prevent penetration, but no forces are computed tangential to the contact surfaces. The string name is a user-selected name for this friction model that is used when identifying this model in the interaction definitions. No command lines are needed inside the command block.

7.11.2 Constant Friction Model

```
BEGIN CONSTANT FRICTION MODEL <string>name
FRICCTION COEFFICIENT = <real>coeff
END [CONSTANT FRICTION MODEL <string>name]
```

The CONSTANT FRICTION MODEL command block defines a constant coulomb friction coefficient between two surfaces as they slide past each other in contact. No resistance is provided to keep the surfaces together if they start to separate. The string name is a user-selected name for this friction model that is used to identify this model in the interaction definitions, and coeff is the constant coulomb friction coefficient. There is no default value for the friction coefficient.
7.11.3  Tied Model

BEGIN TIED MODEL <string>name
END [TIED MODEL <string>name]

The TIED MODEL command block restricts nodes found in initial contact with faces to stay in the same relative location to the faces throughout the analysis. The string name is a user-selected name for this friction model that is used to identify this model in the interaction definitions. No command lines are needed inside the command block.

7.11.4  Spring Weld Model

BEGIN SPRING WELD MODEL <string>name
NORMAL DISPLACEMENT FUNCTION = <string>func_name
NORMAL DISPLACEMENT SCALE FACTOR = <real>scale_factor(1.0)
TANGENTIAL DISPLACEMENT FUNCTION = <string>func_name
TANGENTIAL DISPLACEMENT SCALE FACTOR =
<real>scale_factor(1.0)
FAILURE ENVELOPE EXPONENT = <real>exponent(2.0)
FAILURE DECAY CYCLES = <integer> num_cycles(1)
FAILED MODEL = <string>failed_model_name|FRICITONLESS
(FRICATIONLESS)
END [SPRING WELD MODEL <string>name]

The SPRING WELD MODEL command block defines a contact friction model that, when applied between two contact surfaces, connects a slave node to the nearest point of a corresponding master face with a spring. The spring behavior is defined by a force-displacement curve in the normal and tangential directions. If the motion of the problem generates displacement between the slave node and its corresponding master face and this motion is in purely the normal or tangential direction, the spring will fail once it passes the maximum displacement in the normal and tangential force-displacement curves, respectively. For displacements that include both normal and tangential components, the spring fails according to a failure criterion defined as the sum of the ratios of the normal and tangential components to their maximum values, raised to a power. If the criterion is greater than 1.0, the spring fails. Once the spring fails, its contact forces reduce over a number of load steps, and the contact evaluation reverts to another user-specified friction model (or frictionless contact if not specified).

In the above command block:

- The string name is a user-selected name for this friction model that is used to identify this model in the interaction definitions.

- The normal force-displacement curve is specified by the NORMAL DISPLACEMENT FUNCTION command line, where the string func_name is the name of a function defined in a DEFINITION FOR FUNCTION command line in the domain scope. This function can be scaled by the real
value scale_factor in the NORMAL DISPLACEMENT SCALE FACTOR command line; the default for this factor is 1.0

- The tangential force-displacement curve is specified by the TANGENTIAL DISPLACEMENT FUNCTION command line, where the string func_name is the name of a function defined in a DEFINITION FOR FUNCTION command line in the domain scope. This function can be scaled by the real value scale_factor in the TANGENTIAL DISPLACEMENT SCALE FACTOR command line; the default for this factor is 1.0.

- The real value exponent in the FAILURE ENVELOPE EXPONENT command line specifies how normal and tangential failure criteria may be combined to yield failure of the weld, as described above. The default value for this exponent is 2.0.

- The FAILURE DECAY CYCLES command line describes how many cycles to ramp down the load in the spring weld after it fails through the integer value num_cycles. The default value for the number of decay cycles is 1.

- When the spring weld breaks, the friction model that contact reverts to when evaluating future node-face interactions between the surfaces is identified in the FAILED MODEL command line with the string failed_model_name. The friction model listed in this command must have been previously defined in the input file. The default value for the model used after failure is the frictionless model.

The SPRING WELD MODEL command block is very similar to the Presto SPOT WELD command block, but permits greater flexibility in specifying a different friction model to be applied after failure.

### 7.11.5 Surface Weld Model

BEGIN SURFACE WELD MODEL <string>name
NORMAL CAPACITY = <real>normal_cap
TANGENTIAL CAPACITY = <real>tangential_cap
FAILURE DECAY CYCLES = <integer>num_cycles(1)
FAILED MODEL = <string>failed_model_name|FRICITIONLESS
END [SURFACE WELD MODEL <string>name]

The SURFACE WELD MODEL command block defines a contact friction model that behaves identically to the TIED MODEL until a maximum force between the node and face of an interaction is reached in the normal direction or the tangential direction. Once this maximum force is reached, the tied contact “fails” and the friction model switches to a different friction model, as specified by the user.

In the above command block, the string name is a user-selected name for this friction model that is used to identify this model in the interaction definitions. The maximum allowed force in the normal direction is specified by the real value normal_cap in the NORMAL CAPACITY command line. The
maximum allowed force in the tangential direction is specified by the real value \texttt{tangential\_cap} in the \texttt{TANGENTIAL\_CAPACITY} command line. There are no defaults for these values. The surface weld will break when either the specified normal or tangential capacity is reached. Once the model fails, the applied forces decrease to zero over a number of time steps defined through the integer value \texttt{num\_cycles} in the \texttt{FAILURE\_DECAY\_CYCLES} command line. The default for \texttt{num\_cycles} is 1. The friction model that should be used after the weld fails is identified in the \texttt{FAILED\_MODEL} command line with the string \texttt{failed\_model\_name}. The friction model designated in the \texttt{FAILED\_MODEL} command line must be defined within the \texttt{CONTACT\_DEFINITION} command block. The default model after failure is the frictionless contact model.

#### 7.11.6 Area Weld Model

```
BEGIN AREA WELD MODEL <string>name
    NORMAL CAPACITY = <real>normal\_cap
    TANGENTIAL CAPACITY = <real>tangential\_cap
    FAILURE DECAY CYCLES = <integer> num\_cycles(1)
    FAILED MODEL = <string>failed\_model\_name|FRICTIONLESS
                      (FRICTIONLESS)
END [AREA WELD MODEL <string>name]
```

The \texttt{AREA\_WELD\_MODEL} command block defines a contact friction model that behaves identically to the \texttt{TIED\_MODEL} until a maximum traction between a node and face in an interaction is reached in the normal direction or the tangential direction. Once this maximum traction is reached, the tied contact “fails” and the friction model switches to a different friction model, as specified by the user. This model is identical to the \texttt{SURFACE\_WELD\_MODEL} command block, except that tractions are used instead of forces.

In the above command block, the string \texttt{name} is a user-selected name for this friction model that is used to identify this model in the interaction definitions. The maximum allowed traction in the normal direction is specified by the real value \texttt{normal\_cap} in the \texttt{NORMAL\_CAPACITY} command line. The maximum allowed traction in the tangential direction is specified by the real value \texttt{tangential\_cap} in the \texttt{TANGENTIAL\_CAPACITY} command line. There are no defaults for these values. The area weld will break when either the specified normal or tangential capacity is reached. Once the model fails, the applied tractions decrease to zero over a number of time steps defined through the integer value \texttt{num\_cycles} in the \texttt{FAILURE\_DECAY\_CYCLES} command line. The default for \texttt{num\_cycles} is 1. The friction model that should be used after the weld fails is identified in the \texttt{FAILED\_MODEL} command line with the string \texttt{failed\_model\_name}. The friction model designated in the \texttt{FAILED\_MODEL} command line must be defined within the \texttt{CONTACT\_DEFINITION} command block. The default model after failure is the frictionless contact model.

#### 7.11.7 Adhesion Model

```
BEGIN ADHESION MODEL <string>name
```

In the above command block, the string \texttt{name} is a user-selected name for this friction model that is used to identify this model in the interaction definitions. The maximum allowed traction in the normal direction is specified by the real value \texttt{normal\_cap} in the \texttt{NORMAL\_CAPACITY} command line. The maximum allowed traction in the tangential direction is specified by the real value \texttt{tangential\_cap} in the \texttt{TANGENTIAL\_CAPACITY} command line. There are no defaults for these values. The area weld will break when either the specified normal or tangential capacity is reached. Once the model fails, the applied tractions decrease to zero over a number of time steps defined through the integer value \texttt{num\_cycles} in the \texttt{FAILURE\_DECAY\_CYCLES} command line. The default for \texttt{num\_cycles} is 1. The friction model that should be used after the weld fails is identified in the \texttt{FAILED\_MODEL} command line with the string \texttt{failed\_model\_name}. The friction model designated in the \texttt{FAILED\_MODEL} command line must be defined within the \texttt{CONTACT\_DEFINITION} command block. The default model after failure is the frictionless contact model.
The ADHESION MODEL command block defines a friction model that behaves like frictionless contact when two surfaces are in contact, but computes an additional force between the surfaces when they are not touching. The value of the additional force is given by a user-specified function of force versus distance, where the distance is the distance between a node and the closest point on the opposing surface.

In the above command block, the string name is a user-selected name for this friction model that is used to identify this model in the interaction definitions. The force between surfaces that are not touching is given by the ADHESION FUNCTION command line, where the string func_name is the name of a function defined in a DEFINITION FOR FUNCTION command block in the domain scope. The values of this function are expected to be nonnegative. The function can be scaled by the real value scale_factor in the ADHESION SCALE FACTOR command line; the default for this factor is 1.0. Because contact forces are typically only given to node-face interactions if they touching, the contact search requires appropriate tolerances when this model is used. The normal and tangential tolerances specified in the interaction definitions should be set to the maximum distance at which the adhesion model should be applying force. However, setting this distance to be very large may cause excessive numbers of interactions to be identified in the search phase, causing the contact processing to be very slow and/or generate erroneous interactions.

7.11.8 Cohesive Zone Model

BEGIN COHESIVE ZONE MODEL <string>name
  TRACTION DISPLACEMENT FUNCTION = <string>func_name
  TRACTION DISPLACEMENT SCALE FACTOR = <real>scale_factor(1.0)
  CRITICAL NORMAL GAP = <real>crit_norm_gap
  CRITICAL TANGENTIAL GAP = <real>crit_tangential_gap
END [COHESIVE ZONE MODEL <string>name]

The COHESIVE ZONE MODEL command block defines a friction model that prevents penetration when contact surfaces are touching, but provides an additional force when the distance between the node and face in an interaction increases. This force is determined by a user-specified function. Once the distance exceeds a user-specified value in the normal direction or the tangential direction, the force is no longer applied. This model can be used to mimic the energy required to separate two surfaces that are initially touching.

In the above command block, the string name is a user-selected name for this friction model that is used to identify this model in the interaction definitions. The displacement function for traction is given by the TRACTION DISPLACEMENT FUNCTION command line, where the string func_name is the name of a function defined in a DEFINITION FOR FUNCTION command block in the domain scope. This function can be scaled by the real value scale_factor in the TRACTION DISPLACEMENT SCALE FACTOR command line.
DISPLACEMENT SCALE FACTOR command line; the default for this factor is 1.0. In the CRITICAL NORMAL GAP command line, the real value crit_norm_gap specifies the normal distance between the node and face past which the cohesive zone no longer provides a force. In the CRITICAL TANGENTIAL GAP command line, the real value crit_tangential_gap specifies the tangential distance between the node and face past which the cohesive zone no longer provides a force.

7.11.9 Junction Model

BEGIN JUNCTION MODEL <string>name
   NORMAL TRACTION FUNCTION = <string>func_name
   NORMAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
   TANGENTIAL TRACTION FUNCTION = <string>func_name
   TANGENTIAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
   NORMAL CUTOFF DISTANCE FOR TANGENTIAL TRACTION = <real>distance
END [JUNCTION MODEL <string>name]

The JUNCTION MODEL command block defines a model that prevents the interpenetration of contact surfaces and that also provides normal and tangential tractions to a node-face interaction when the surfaces are not touching. The normal tractions are defined as a function of the normal distance between the node and face of an interaction, while the tangential traction is given as a function of the relative tangential velocity. The tractions are defined by user-specified functions, and the tangential tractions from this model drop to zero once the normal distance between the node and the face exceeds a critical value. This friction model provides a simple way to model threaded connections, though the THREADED MODEL defined in Section 7.11.10 has more flexibility.

In the above command block, the string name is a user-selected name for this friction model that is used to identify this model in the interaction blocks. The normal traction curve is specified by the NORMAL TRACTION FUNCTION command line, where the string func_name is the name of a function defined in a DEFINITION FOR FUNCTION command block in the domain scope. This function defines a relation between the traction and the distance between the node and the face in the normal direction. This function can be scaled by the real value scale_factor in the NORMAL TRACTION SCALE FACTOR command line; the default for this factor is 1.0. Similarly, the tangential traction curve is specified by the TANGENTIAL TRACTION FUNCTION command line, where the string func_name is the name of a function defined in a DEFINITION FOR FUNCTION command block in the domain scope. This function defines a relation between the traction and the relative velocity of the node and face in the tangential direction. This function can be scaled by the real value scale_factor in the TANGENTIAL TRACTION SCALE FACTOR command line; the default for this factor is 1.0. Once the normal distance between a node and a face using this model reaches a critical distance, the tangential traction drops to zero; this distance is specified with the real value distance in the NORMAL CUTOFF DISTANCE FOR TANGENTIAL TRACTION command line.
7.11.10 Threaded Model

BEGIN THREADED MODEL <string>name
    NORMAL TRACTION FUNCTION = <string>func_name
    NORMAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
    TANGENTIAL TRACTION FUNCTION = <string>func_name
    TANGENTIAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
    TANGENTIAL TRACTION GAP FUNCTION = <string>func_name
    TANGENTIAL TRACTION GAP SCALE FACTOR = <real>scale_factor(1.0)
    NORMAL CAPACITY = <real>normal_cap
    TANGENTIAL CAPACITY = <real>tangential_cap
    FAILURE ENVELOPE EXPONENT = <real>exponent(2.0)
    FAILURE DECAY CYCLES = <integer>num_cycles(1)
    FAILED MODEL = <string>failed_model_name|FRICITIONLESS
        (FRICITIONLESS)
END [THREADED MODEL <string>name]

The **THREADED MODEL** command block defines a friction model that is designed to mimic a threaded interface. This model prevents interpenetration of contact surfaces, and also supplies additional tractions when the surfaces are not touching. Tensile tractions in the normal direction are given by a user-specified function of force versus distance between the node and face. Tensile tractions in the tangential direction are computed as the product of a traction tangential-displacement curve and a scaling curve that is a function of the normal displacement. Maximum normal and tangential tractions are input such that the model “fails” at a node-face interaction once they are reached. For interactions that include both normal and tangential displacements, the model failure is defined according to a failure criterion defined as the sum of the ratios of the normal and tangential traction components to their maximum capacity values, raised to a power. After failure, interactions shift to a different user-specified friction model.

In the above command block:

- The string **name** is a user-selected name for this friction model that is used to identify the model in the interaction definitions.

- The traction-displacement relation in the normal direction is specified by the **NORMAL TRACTION FUNCTION** command line, where the string **func_name** is the name of a function defined in a **DEFINITION FOR FUNCTION** command block in the domain scope. This function can be scaled by the real value **scale_factor** in the **NORMAL TRACTION SCALE FACTOR** command line; the default for this factor is 1.0.

- The traction-displacement relation in the tangential direction is specified by two curves. The traction-displacement relation in the tangential direction when there is no displacement in the normal direction is defined by the **TANGENTIAL TRACTION FUNCTION** command line, where the string **func_name** is the name of a function defined in a **DEFINITION FOR FUNCTION** command block in the domain scope. This function can be scaled by the real value **scale_factor** in the **TANGENTIAL TRACTION SCALE FACTOR** command line; the
default for this factor is 1.0. When the distance in the normal direction is greater than zero, the tangential traction is scaled by a function specified in the TANGENTIAL TRACTION GAP FUNCTION command line, where the string func_name is the name of a function defined in a DEFINITION FOR FUNCTION command block in the domain scope. This function defines a scaling factor as a function of the normal displacement. The function can be scaled by the real value scale_factor in the TANGENTIAL TRACTION GAP SCALE FACTOR command line; the default for this factor is 1.0.

- The threaded model “fails” once the normal and tangential tractions reach a critical capacity value. The normal capacity is specified by the real value normal_cap in the NORMAL CAPACITY command line. The tangential capacity is specified by the real value tangential_cap in the TANGENTIAL CAPACITY command line. There are no default values for these parameters. These capacities are defined for pure normal or tangential displacements. In cases where there is a combination of tangential and normal displacements, a failure curve is used to determine the combination of tangential and normal tractions that determines model failure. This curve is defined as the sum of the ratios of the normal and tangential traction components to their maximum capacity values, raised to a power. The power in the function is defined by the real value exponent in the FAILURE ENVELOPE EXPONENT command line. The default value of the exponent is 2.0. Once the model fails, the applied tractions decrease to zero over a number of time steps defined through the integer value num_cycles in the FAILURE DECAY CYCLES command line. The default for num_cycles is 1. When the model exceeds the designated capacity, the contact surfaces using this model switch to a different friction model as identified in the FAILED MODEL command line with the string failed_model_name. The friction model designated in the FAILED MODEL command line must be defined within the CONTACT DEFINITION command block. The default model is the frictionless model.

### 7.11.11 PV_Dependent Model

BEGIN PV_DEPENDENT MODEL <string>name
  STATIC COEFFICIENT = <real>stat_coeff
  DYNAMIC COEFFICIENT = <real>dyn_coeff
  VELOCITY DECAY = <real>vel_decay
  REFERENCE PRESSURE = <real>p_ref
  OFFSET PRESSURE = <real>p_off
  PRESSURE EXPONENT = <real>p_exp
END [PV_DEPENDENT MODEL <string> name]

The PV_DEPENDENT MODEL command block defines a friction model similar to a coulomb friction model, but which provides a frictional response that is dependent on the pressure and the velocity. The pressure-dependent portion of the model behaves similarly to the constant friction model except that the tangential traction is given by

$$
\left[ \frac{p + p_{\text{off}}}{p_{\text{ref}}} \right]^{p_{\exp}}.
$$

(7.1)
The velocity-dependent part is given by

\[(stat\_coeff - dyn\_coeff) e^{-(vel\_decay \|v\|)} + dyn\_coeff.\]  \hspace{1cm} (7.2)

The `PV\_DEPENDENT\_MODEL` command block multiplies the pressure and velocity effects together. In the above command block:

- The string `name` is a name assigned to this friction model that is used to identify the model in the interaction definitions.
- The real value `p\_ref` in the pressure-dependent part given in Equation (7.1) is specified with the `REFERENCE\_PRESSURE` command line.
- The real value `p\_off` in the pressure-dependent part given in Equation (7.1) is specified with the `OFFSET\_PRESSURE` command line.
- The real value `p\_exp` in the pressure-dependent part given in Equation (7.1) is specified with the `PRESSURE\_EXponent` command line.
- The real value `stat\_coeff` in the velocity-dependent part given in Equation (7.2) is specified with the `STATIC\_COEFFICIENT` command line.
- The real value `dyn\_coeff` in the velocity-dependent part given in Equation (7.2) is specified with the `DYNAMIC\_COEFFICIENT` command line.
- The real value `vel\_decay` in the velocity-dependent part given in Equation (7.2) is specified with the `VELOCITY\_DECAY` command line.

### 7.11.12 User Subroutine Friction Models

```plaintext
BEGIN USER SUBROUTINE MODEL <string>name
    INITIALIZE MODEL SUBROUTINE = <string>init_model_name
    INITIALIZE TIME STEP SUBROUTINE = <string>init_ts_name
    INITIALIZE NODE STATE DATA SUBROUTINE = <string>init_node_data_name
    LIMIT FORCE SUBROUTINE = <string>limit_force_name
    ACTIVE SUBROUTINE = <string>active_name
    INTERACTION TYPE SUBROUTINE = <string>interaction_name
END [USER SUBROUTINE MODEL <string>name]
```

The `USER\_SUBROUTINE\_MODEL` command blocks permit contact to use a user subroutine to define a friction model between surfaces. This capability is in a test phase at this time; please contact a Presto developer for more information.

In this command block:
- The string name is a user-specified name that is used to identify this model in the interaction definitions.

- The command line INITIALIZE MODEL SUBROUTINE specifies a user subroutine to initialize the friction model. The name of the subroutine is given by init_model_name.

- The command line INITIALIZE TIME STEP SUBROUTINE specifies a user subroutine to initialize the time step. The name of the subroutine is given by init_ts_name.

- The command line INITIALIZE NODE STATE DATA SUBROUTINE specifies a user subroutine to initialize the node state data. The name of the subroutine is given by init_node_data_name.

- The command line LIMIT FORCE SUBROUTINE specifies a user subroutine to provide the limit force for the friction model. The name of the subroutine is given by limit_force_name.

- The command line ACTIVE SUBROUTINE specifies a user subroutine to compute forces for an active node-face interaction. The name of the subroutine is given by active_name.

- The command line INTERACTION TYPE SUBROUTINE specifies a user subroutine to define the interaction type. The name of the subroutine is given by interaction_name.


7.12 Search Options

BEGIN SEARCH OPTIONS [<string>name]

# search algorithms
GLOBAL SEARCH INCREMENT = <integer>num_steps(1)
GLOBAL SEARCH ONCE = <string>ON|OFF(OFF)
#
# search tolerances
SEARCH TOLERANCE = <string>AUTOMATIC|USER_DEFINED
(AUTOMATIC)
NORMAL TOLERANCE = <real>norm_tol
TANGENTIAL TOLERANCE = <real>tang_tol
#
# secondary decomposition
SECONDARY DECOMPOSITION = <string>ON|OFF(OFF)
END [SEARCH OPTIONS <string>name]

For this section, the command usage conforms to the 2.9 release of Presto.

Contact involves a search phase and an enforcement phase. The contact search algorithm used to detect interactions between contact surfaces is often the most computationally expensive part of an analysis. The user can exert some control over how the search phase is carried out via the SEARCH OPTIONS command block. By selecting different options in this command block, the user can make trade-offs between the accuracy of the search and computing time.

The most accurate approach to the search phase is a global search at every time step. For a global search, a box is drawn around each face. The box depends on the shape of the face, the location of the face in space, and search tolerances. Now suppose we want to determine whether some node has penetrated that face. We must first determine if the node lies in one or more boxes that surround a face. This search, although done with an optimal algorithm, is still time consuming. The search must be done for all nodes that may be in contact with a face. A less accurate approach for the search phase is to use what is called a local tracking algorithm. For the tracking algorithm approach, we first do a global search. When a node has contacted a face in the global search, we record the face (or faces) contacted by the node. Instead of using the global search on subsequent time steps, we simply rely on the record of the node-face interactions to compute the contact forces. The last face contacted by a node in the global search is assumed to remain in contact with that node for subsequent time steps. In actuality, the node may slide off the face it was contacting at the time of the global search. In this case, faces that share an edge with the original contact face are searched to determine whether they (the edge adjacent faces) are in contact with the node. If the node moves across a corner of the face (rather than an edge), we may lose the contact interaction for the node until the next global search. If we lose the contact interaction, we lose some of the accuracy in the contact calculations until we do the next global search. Furthermore, it is possible that additional nodes may actually come into contact in the time steps between global searches. These nodes are typically caught during the next global search, but inaccuracies can result from missing the exact time of contact. The tracking algorithm, under certain circumstances, can work quite well even though it is less accurate. We can encounter analyses where we can set the number of intervals (time steps) between global searches to a relatively small number (5) and lose only
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a few or none of the node-to-face contacts between global searches. Likewise, we can encounter analyses where we can set the interval between global searches to a large number (100 or more) and lose only a few or none of the node-to-face contacts between global searches. Finally, we can encounter problems where we may only have to do one global search at the beginning and rely solely on the tracking information for the rest of the problem (without losing any contact). What search approach is best for your problem depends on the geometry of your structure, the loads on your structure, and the amount of deformation of your structure. This section tells you how to control the search phase for your specific problem.

The SEARCH OPTIONS command block begins with the input line:

    BEGIN SEARCH OPTIONS [<string>name]

and ends with:

    END [SEARCH OPTIONS <string>name]

The name for the command block is optional.

Without a SEARCH OPTIONS command block, the default search with associated default search parameters is used for all contact pairs. If you want to override the default search method for all contact pairs, you should add a SEARCH OPTIONS command block. By adding a SEARCH OPTIONS command block, you establish a new set of global defaults for the search for all contact pairs. The default for the search is that tracking is turned on and the number of intervals (time steps) between a global search is one (GLOBAL SEARCH INCREMENT = 1 and GLOBAL SEARCH ONCE = OFF).

The valid command lines within a SEARCH OPTIONS command block are described in Section 7.12.1, Section 7.12.2, and Section 7.12.3. The values specified by these commands are applied by default to all interaction contact surfaces, unless overridden by a specific interaction definition.

7.12.1 Search Algorithms

    GLOBAL SEARCH INCREMENT = <integer>num_steps(1)
    GLOBAL SEARCH ONCE = <string>ON|OFF(OFF)

The above two command lines let you determine the frequency of the global search. Although these command lines are mutually exclusive, they provide for three search options:

1. If you want to do only one global search and have all subsequent searches be tracking searches, then you should use the GLOBAL SEARCH ONCE command line with the string parameter set to ON. By default, the GLOBAL SEARCH ONCE option is OFF. If you set GLOBAL SEARCH ONCE to ON, then this should be the only command line for the search algorithms in the command block. The GLOBAL SEARCH INCREMENT command line should not be used.

2. If you want to use the global search only intermittently, with the tracking search in between the global search, you should use the GLOBAL SEARCH INCREMENT set to some integer
value greater than 1. The integer value \textit{num\_steps} determines the number of time steps between global searches. The \texttt{GLOBAL SEARCH ONCE} command line should not be used.

3. If you want to do a global search at every time step, you should use the \texttt{GLOBAL SEARCH INCREMENT} command line with \textit{num\_steps} set to 1 or just simply omit this line since the default for the search increment is 1. The \texttt{GLOBAL SEARCH ONCE} command line should not be used.

In summary, you have three options for the global search. You can do a global search only once (the first time step), and do a tracking search for all subsequent searches by setting \texttt{GLOBAL SEARCH ONCE} to \texttt{ON}. You can do a global search for the beginning time step and intermittently thereafter; the time steps between the global searches will use a tracking search. For this approach, you will need only the \texttt{GLOBAL SEARCH INCREMENT} command line. Finally, you can set \texttt{GLOBAL SEARCH INCREMENT} to 1 and do a global search at every time step.

### 7.12.2 Search Tolerances

\begin{verbatim}
SEARCH TOLERANCE = <string> AUTOMATIC | USER_DEFINED(AUTOMATIC)
NORMAL TOLERANCE = <real> norm_tol
TANGENTIAL TOLERANCE = <real> tang_tol
\end{verbatim}

As indicated previously, the contact functionality in Presto uses a box defined around each face to locate nodes that may potentially contact the face. This box is defined by a tolerance normal to the face and another tolerance tangential to the face (see Figure 7.4). The code adds to these tolerances the maximum motion over a time step when identifying interactions. In the above command lines, the parameter \textit{norm\_tol} is the normal tolerance (defined on the \texttt{NORMAL TOLERANCE} command line) for the search box and the parameter \textit{tang\_tol} is the tangential tolerance (defined on the \texttt{TANGENTIAL TOLERANCE} command line) for the search box.

By default, Presto will automatically calculate normal and tangential tolerances. The default value for the command line \texttt{SEARCH TOLERANCE} is \texttt{AUTOMATIC}. If you leave automatic search on and also specify normal and/or tangential tolerances with the \texttt{NORMAL TOLERANCE} and \texttt{TANGENTIAL TOLERANCE} command lines, the larger of the two (automatic or user specified) tolerances will be used. For example, suppose you specify a normal tolerance of $1.0 \times 10^{-3}$ and the automatic tolerancing computes a normal tolerance of $1.05 \times 10^{-3}$. Then Presto will use a normal tolerance of $1.05 \times 10^{-3}$.

\begin{attention}
\textbf{Known Issue:} Automatic search tolerances is a new capability and some users have reported issues with this in their initial testing. Using normal and tangential tolerances is recommended until these issues are sorted out.
\end{attention}

When the \texttt{USER_DEFINED} option is specified for the \texttt{SEARCH TOLERANCE} command line, these normal and tangential tolerances must be specified. If these tolerances are not specified, code execution will be terminated with an error.
Both of these tolerances are absolute distances in the same units as the analysis. The proper tolerances are problem dependent. If a normal or tangential tolerance is specified in the SEARCH OPTIONS command block, they apply to all interactions. These default search tolerances can be overwritten for a specific interaction by specifying a value for the normal tolerance and/or tangential tolerance for that interaction inside the INTERACTION command block (see Section 7.15).

7.12.3 Secondary Decomposition

SECONDARY DECOMPOSITION = <string>ON|OFF(ON)

The SECONDARY DECOMPOSITION command line controls internal options used by the ACME contact search algorithm. Computational results for secondary decomposition ON should be identical to those for secondary decomposition OFF. However, the computational time for these two distinct options may vary significantly.

When a mesh is divided for parallel processing, it is usually divided such that each processor has the same number of elements. The element-based load balance needs to achieve good parallel performance for element and material calculations. It is possible to have the number of elements per processor balanced but the number of contact faces per processor highly unbalanced. If contact is highly localized in one region of the model, it may happen that a small subset of the processors contains most of the contact interactions. A secondary decomposition is a parallel decomposition that balances the number of contact faces. When secondary decomposition is on, the contact algorithm first moves all data to the secondary decomposition and then it runs the contact calculations. When the secondary decomposition is off, all contact calculations are done in the primary decomposition.

The computational effort to move data to the secondary decomposition can be quite large. Thus, if the contact surfaces are well balanced in the primary decomposition, a large cost savings can be realized by turning off the secondary decomposition. Three conditions must be met for turning off the secondary decomposition to achieve cost savings. First, the number of contact faces per processor must be somewhat balanced in the primary decomposition. Second, faces in contact
should be on the same processor as much as possible. Inertial and RCB decomposition tend to meet this condition of having contact faces in proximity on the same processor, while Multi-KL does not. Third, conditions one and two must persist throughout the entire analysis. An initially well balanced, well distributed mesh may become poorly balanced through element death or large deformations.

The best recommendation is to leave the secondary decomposition on.
7.13 Enforcement Options

BEGIN ENFORCEMENT OPTIONS [<string>name]
   ENFORCEMENT ALGORITHM = <string>MOMENTUM_BALANCE|
   PENALTY(MOMENTUM_BALANCE)
   MOMENTUM BALANCE ITERATIONS = <integer>num_iterations(5)
END [ENFORCEMENT OPTIONS <string>name]

Contact, as previously indicated, involves a search phase and an enforcement phase. The user can exert some control over how the enforcement phase is carried out via the ENFORCEMENT OPTIONS command block. By selecting different options in this command block, the user can make trade-offs between solution accuracy and computing time. The ENFORCEMENT OPTIONS command block begins with the input line:

BEGIN ENFORCEMENT OPTIONS [<string>name]

and is terminated with the input line:

END [ENFORCEMENT OPTIONS <string>name]

The name for the command block, name, is optional.

Only a single ENFORCEMENT OPTIONS command block is permitted within a CONTACT DEFINITION command block. Without an ENFORCEMENT OPTIONS command block, the default enforcement algorithm with associated default enforcement options is used for all contact pairs. If you want to override the defaults for enforcement for all contact pairs, you should add an ENFORCEMENT OPTIONS command block. By adding this command block, you establish a new set of global defaults for enforcement for all contact pairs. You can override some of these global defaults for enforcement for a contact pair by inserting certain command lines in the INTERACTION command block (see Section 7.15) for that contact pair. It is possible, therefore to tailor the enforcement approach for individual contact pairs.

Currently, the enforcement option is of limited use. Options for user control will be expanded in future versions of Presto.

The ENFORCEMENT ALGORITHM command line lets the user select either a momentum balance enforcement algorithm (MOMENTUM_BALANCE) or a penalty method enforcement algorithm (PENALTY). The default value is MOMENTUM_BALANCE.

For the current release of Presto users should rely on the default enforcement algorithm, the momentum balance approach. Consult with a Presto developer if you would like to use the penalty method.

The momentum balance algorithm for enforcement of the contact constraints uses an iterative process to ensure incremental momentum balance over a time step. Rather than making one pass to compute contact forces for node push-back, several passes are made to more accurately compute the normal contact force and, subsequently, the tangential (frictional) contact forces. The number of passes (iterations) is set by the value num_iterations in the MOMENTUM BALANCE ITERATIONS command line. The default value for the number of iterations is 5. This value is generally acceptable for removing overlap in the mesh. To get accurate results in a global sense...
in analyses that use friction, a value of 10 is more appropriate. To get accurate contact response at individual points in analyses with friction, a value of 20 or greater may be needed. Note that as the number of iterations increases, the expense of enforcement increases. Thus a user can balance execution speed and accuracy with this command line, though care must be taken to ensure that the appropriate level of accuracy is attained. This command line affects only the enforcement phase of the contact. A single search phase is used for contact detection, but the enforcement phase uses an iterative process.
7.14 Default Values for Interactions

BEGIN INTERACTION DEFAULTS [<string>name]
SURFACES = <string list>surface_names
SELF CONTACT = <string>ON|OFF(OFF)
GENERAL CONTACT = <string>ON|OFF(OFF)
AUTOMATIC KINEMATIC PARTITION = <string>ON|OFF(OFF)
FRICITION MODEL = <string>friction_model_name|FRICTIONLESS (FRICTIONLESS)
INTERACTION BEHAVIOR = <string>SLIDING|INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)
END [INTERACTION DEFAULTS <string>name]

For this section, the command usage conforms to the 2.9 release of Presto.

This section discusses the INTERACTION DEFAULTS command block. Note that the name for the INTERACTION DEFAULTS command block, name, is currently not used or required. This command block lets you enforce contact on a subset of all contact surfaces or on all contact surfaces. You may overwrite predefined values defining surface interaction (for all surfaces defined by this command block) by using several different command lines.

It is important to note that unless some combination of the INTERACTION DEFAULTS command block and INTERACTION command blocks (Section 7.15) exists in the CONTACT DEFINITION command block, enforcement will not take place. Up to this point, all command lines and command blocks have provided information to set up the search phase and have provided details for surface interaction. However, contact enforcement for surfaces—the actual removal of interpenetration between surfaces and the calculation of surface forces consistent with friction models—will not take place unless some combination of the INTERACTION DEFAULTS command block and INTERACTION command blocks is used to set up surface interactions.

Contact between surfaces requires data to describe the interaction between these surfaces. You may specify defaults for the surface interactions for some or all surface pairs by using the INTERACTION DEFAULTS command block. Within this command block, you can provide a list of surfaces that are a subset of the contact surfaces. Any pair of surfaces listed in the INTERACTION DEFAULTS command block will acquire the default values that are defined within the INTERACTION DEFAULTS command block. If you omit the SURFACES command line, defaults in the INTERACTION DEFAULTS command block are applied to all surfaces. Any default set within an INTERACTION DEFAULTS command block can be overridden by commands in an INTERACTION command block. See Section 7.15.

If you consider only the use of the INTERACTION DEFAULTS command block (and not the use of the INTERACTION command block), you have three options for the surface interaction values:

- You can specify default surface interaction values for all the contact surface pairs by specifying all the contact surfaces in an INTERACTION DEFAULTS command block.
- You can specify default surface interaction values for some of the contact surface pairs by specifying a subset of the contact surfaces in an INTERACTION DEFAULTS command block.
You can leave all interactions off by default by not specifying an \texttt{INTERACTION DEFAULTS} command block.

You can overwrite surface interaction values that you have set with an \texttt{INTERACTION DEFAULTS} command block by using an \texttt{INTERACTION} command block.

The valid commands within an \texttt{INTERACTION DEFAULTS} command block are described in Section 7.14.1 through Section 7.14.5. The values specified by the command lines in the \texttt{INTERACTION DEFAULTS} command block are applied by default to all interaction contact surfaces unless overridden by a specific interaction definition.

\subsection*{7.14.1 Surface Identification}

\begin{verbatim}
SURFACES = <string list>surface_names
\end{verbatim}

This command line identifies the contact surfaces to which the surface interaction values defined in the \texttt{INTERACTION DEFAULTS} command block will apply. The string list on the \texttt{SURFACES} command line specifies the names of these contact surfaces. The \texttt{SURFACES} command line can include any surface specified in a \texttt{CONTACT SURFACE} command line, a \texttt{CONTACT SURFACE} command block, or a \texttt{SKIN ALL BLOCKS} command line.

The \texttt{SURFACES} command line is optional. If you want the defaults to apply to all the surfaces you have defined, you will NOT use the \texttt{SURFACES} command line in this command block. If you want the defaults to apply to a subset of all contact surfaces, then you will list the specific set of surfaces on a \texttt{SURFACES} command line. The names of all the surfaces with the default values will be listed in the string list designated as \texttt{surface_names}.

\subsection*{7.14.2 Self-Contact and General Contact}

\begin{verbatim}
SELF CONTACT = <string>ON\mid OFF\hspace{1em}(OFF)
GENERAL CONTACT = <string>ON\mid OFF\hspace{1em}(OFF)
\end{verbatim}

The \texttt{SELF CONTACT} command line, if set to \texttt{ON}, specifies that the default values set in the command lines of the command block will apply to self-contact between the listed surfaces (or all surfaces if no surfaces are listed). The \texttt{GENERAL CONTACT} command line, if set to \texttt{ON}, specifies that the default values set in the command lines of this command block apply to contact between the listed surfaces (or all surfaces if no surfaces are listed) excluding self-contact. The default values for both of these command lines is \texttt{OFF}. If you want to enforce general contact between all surfaces specified in the \texttt{INTERACTION DEFAULTS} command block but no self-contact, you must include the line:

\begin{verbatim}
GENERAL CONTACT = ON
\end{verbatim}

If you want to enforce self-contact for all surfaces specified in the \texttt{INTERACTION DEFAULTS} command block, you must include the line:
SELF CONTACT = ON

Suppose that you have only an interaction defaults command block with no interaction command block in your contact definition command block. Unless you have a general contact command line set to on, a self contact command line set to on, or both the general contact command line set to on and the self contact command line set to on, no enforcement will occur.

Suppose you have turned on contact enforcement for all contact surface pairs (general contact and self-contact) in the interaction defaults command block. You may turn off contact enforcement for a specific contact pair by use of the interaction behavior command line in the interaction command block. (The same holds true if you have turned on contact enforcement for only a subset of contact surface pairs in the interaction defaults command block.)

Suppose you have turned on self-contact enforcement for all contact surfaces in the interaction defaults command block. You may override self-enforcement for a specific contact surface by use of the interaction behavior command line in the interaction command block. (The same holds true if you have turned on contact enforcement for only a subset of contact surfaces in the interaction defaults command block.)

7.14.3 Friction Model

\[ \text{FRICTION MODEL} = \langle \text{string}\rangle \text{friction_model_name}\mid \text{FRICTIONLESS} \]

:The friction model command line permits the description of how surfaces interact with each other using a friction model defined in a friction-model command block (see Section 7.11). In the above command line, the string friction_model_name should match the name assigned to some friction model command block. For example, if you specified the name of an area weld command block as AW1 and wanted to reference that name in the friction model command line, the value of friction_model_name would be AW1.

The default interaction is frictionless contact.

7.14.4 Automatic Kinematic Partition

\[ \text{AUTOMATIC KINEMATIC PARTITION} \]

If the automatic kinematic partition command line is used, Presto will automatically compute the kinematic partition factors for pairs of surfaces. (See Section 7.15.2 for more information on kinematic partitioning.) The automatic kinematic partitions are computed from the impedance of each surface based on nodal average density and wave speed. Automatic computation of kinematic partition factors provides the best approach to exact enforcement of symmetric contact of opposing surfaces provided that these surfaces have the same mesh resolution. If the mesh resolution is disparate, you can specify the coarser meshed body as master, but generally it is better to use more contact iterations to deal with this case of a fine mesh contacting a coarse mesh.
For the interaction of any two surfaces, the sum of the partition factors for the surfaces must be 1.0. This is automatically taken care of when the AUTOMATIC KINEMATIC PARTITION command line is used. The default value for kinematic partition factors for all surfaces is 0.5.

The AUTOMATIC KINEMATIC PARTITION command line can be used to set the kinematic partitions for all interactions or to set the kinematic partitions for specific interactions. Thus the command line can appear in two different scopes:

1. The command line can be used within the INTERACTION DEFAULTS command block. In this case, all contact surface interactions defined in the command block will use the automatic kinematic partitioning scheme by default. This will override the default case that assigns a kinematic partition factor of 0.5 to all surfaces. For particular interactions, it is possible to override the use of the automatic kinematic partition factors by specifying kinematic partition values (with the KINEMATIC PARTITION command line) within the INTERACTION command blocks for those interactions.

2. The command line can be used inside an INTERACTION command block. If the automatic partitioning command line appears inside an INTERACTION command block, the kinematic partition factors for that particular interaction will be calculated by the automatic kinematic partition scheme.

Automatic kinematic partitioning is not currently operational for shell elements. If it is enabled, the kinematic partitioning factor is set to 0.5 for all contact interactions involving shell elements.

### 7.14.5 Interaction Behavior

\[
\text{INTERACTION BEHAVIOR} = \text{<string>SLIDING|INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)}
\]

The INTERACTION BEHAVIOR command line specifies how the search will be done. For SLIDING contact, the search algorithm is constantly updating information that lets the code accurately track the sliding of the node over the face and any adjacent faces. The SLIDING option, which is the default, lets us handle the case where we have large relative sliding between a face and a node. A node contacting a face can slide over time by a significant amount over the face. The node can slide onto an adjacent face or onto a face on a nearby surface. For the case of INFINITESIMAL_SLIDING, search information is not updated to the extent that it is with the SLIDING option. In the case of INFINITESIMAL_SLIDING, it is assumed that there is very little slip over time of a node relative to its initial contact point on a face. Furthermore, it is assumed a node will not slide off the face that it initially contacts. The INFINITESIMAL_SLIDING option is not as accurate as the SLIDING option, but neither is it as expensive as the SLIDING option. For some cases, however, the INFINITESIMAL_SLIDING option may work quite well even though it is not as accurate as the SLIDING option. Finally, you may turn off the search completely by using the NO_INTERACTION option.
With the third option, NO_INTERACTION, you could turn off the search for all surfaces specified in the INTERACTION DEFAULTS command block. You could then turn on the search on a case-by-case basis for various contact pairs or for the self-contact of surfaces by using INTERACTION command blocks. This is a convenient way to set defaults for the friction model and automatic kinematic partitioning without turning on all the interactions. More likely, you will set contact interactions to default to the SLIDING option in the INTERACTION DEFAULTS command block, and then turn off specific contact interactions through INTERACTION command blocks.

Using the INTERACTION BEHAVIOR command line in the INTERACTION DEFAULTS command block represents a sophisticated application of this command line. Please consult with Presto developers for more information about this command line if it is used in an INTERACTION DEFAULTS command block.
7.15 Values for Specific Interactions

BEGIN INTERACTION [<string>name]
  SURFACES = <string>surface1 <string>surface2
  MASTER = <string>surface
  SLAVE = <string>surface
  KINEMATIC PARTITION = <real>kin_part
  NORMAL TOLERANCE = <real>norm_tol
  TANGENTIAL TOLERANCE = <real>tang_tol
  OVERLAP NORMAL TOLERANCE = <real>over_norm_tol
  OVERLAP TANGENTIAL TOLERANCE = <real>over_tang_tol
  FRICTION MODEL = <string>friction_model_name|FRICIONLESS(FRICTIONLESS)
  AUTOMATIC KINEMATIC PARTITION
  INTERACTION BEHAVIOR = <string>SLIDING|INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)
END [INTERACTION <string>name]

The Presto contact input also permits the setting of values for specific interactions using the INTERACTION command block. If an INTERACTION DEFAULTS command block is present within a CONTACT DEFINITION command block, the values provided by an INTERACTION command block override the defined defaults. If an INTERACTION DEFAULTS command block is not present, only those interactions defined by INTERACTION command blocks are searched for contact, and values without system defaults must be specified.

The INTERACTION command block begins with:

BEGIN INTERACTION [<string>name]

and ends with:

END [INTERACTION <string>name]

where name is a name for the interaction. Note that this name is currently not used or required.

The valid commands within an INTERACTION command block are described in Section 7.15.1 through Section 7.15.6.

7.15.1 Surface Identification

SURFACES = <string>surface1 <string>surface2

MASTER = <string>surface
SLAVE = <string>surface

There are two methods to identify the surfaces described by a specific interaction. The standard method is to identify both surfaces in a single line with the SURFACES command line, where surface1 and surface2 are the names of the two contact surfaces to which the interaction
refers. In this syntax, the values supplied for the interaction are defined for two-way contact, where contact is evaluated twice: once with the first surface as master and the second as slave, and once with the opposite arrangement. How the two contact enforcements are combined is defined with the KINEMATIC PARTITION command line (see Section 7.15.2). Two-way contact provides better-quality contact results for most problems.

To specify one-way contact, where the nodes of the “slave” surfaces are searched against the “master” surface, use the MASTER and SLAVE command lines, where surface is the name of a contact surface defined in the CONTACT DEFINITION command block (see Section 7.2). In this case, all interaction values specified in this command block are applied only to nodes of the slave surface interacting with faces of the master surface. You cannot specify two master-slave interactions in which the contact surfaces are switched. You also cannot specify a kinematic partition for a master-slave interaction; it is assumed to be 1.0.

In the INTERACTION command block, either the SURFACES syntax (SURFACES command line only) or the MASTER/SLAVE syntax (MASTER and SLAVE command lines) should be used, but not both.

For self-contact, use the SURFACES command lines. The two surfaces given in the SURFACES command line are the same contact surface.

### 7.15.2 Kinematic Partition

KINEMATIC PARTITION = <real>kin_part

To provide accurate contact evaluation, Presto typically computes two-way contact between two surfaces, where interactions are defined between the nodes of the first surface and the faces of the second surface, and also between the nodes of the second surface and the faces of the first surface. If the two surfaces have penetrated each other by a distance $\delta$, then each of the contact evaluations will compute forces to move the surface a distance $\delta$, so that the total resulting displacement would be $2\delta$ if both sets of contact computations were fully applied. The KINEMATIC PARTITION command line defines a kinematic partition scaling factor, $\text{kin\_part}$, for the two contact computations so that the total contact motion is correct. The kinematic partition factor, $\text{kin\_part}$, is a value between 0.0 and 1.0. The factor scales the relative motion of the first surface, where $\text{kin\_part} = 0.0$ means the first surface will move none of $\delta$, while $\text{kin\_part} = 1.0$ means the surface moves all of $\delta$. The second surface moves the portion of $\delta$ that remains after the motion of the first surface (i.e., $\delta$ for second surface = $1.0 - \text{kin\_part}$). For instance, if $\text{kin\_part}$ is 0.2, the first surface will move 20% of the penetration distance ($0.2\delta$ in our example), and the second surface would move the remaining 80% ($0.8\delta$ in our example). The default value is 0.5, so that each surface would move half of the penetration distance. If $\text{kin\_part}$ is 0.0, the first surface does not move at all, and the second surface moves the full distance. This is exactly equivalent to a one-way master-slave contact definition, where the first surface is the master and the second is the slave. If $\text{kin\_part}$ is 1.0, the second surface is the master, and the first surface is the slave. Figure 7.5 illustrates how the kinematic partition factor varies from 0.0 to 1.0, with the specific example of $\text{kin\_part}$ being set to 0.2.
The capability provided by the KINEMATIC PARTITION command line is important in cases where contact occurs between two materials of disparate stiffness. Physically, we would expect a material with a higher stiffness to have more of an effect in determining the position of the contact surface than a more compliant material. In this case, we want the softer material to move more of the distance, and thus it should have a higher kinematic partition factor. The appropriate kinematic partition factor can be determined in closed form; see the ACME contact library reference [1] for more information. Alternately, the AUTOMATIC KINEMATIC PARTITION capability can automatically calculate the proper kinematic partition based on the stiffness of the materials.

Another case where the kinematic partition factor has traditionally been used is when meshes with dissimilar resolutions contact each other. If an interaction is defined with a fine mesh as the master surface and a coarse mesh as a slave surface, the contact algorithms will permit nodes on the master surface to penetrate the slave surface. In these cases, such problems can be alleviated by making the coarse mesh the master surface. However, the iterative approach implemented in the enforcement can also take care of this problem and is advised. If very few iterations are chosen, an appropriate kinematic partition factor may be needed to prevent unintentional penetration due to mesh discretization.

For self-contact, the kinematic partition factor should be 0.5.

A kinematic partition factor cannot be defined for interactions that use the pure master-slave syntax (see Section 7.15.1).

In general, it is best to use the automatic kinematic partition option to properly compute the kinematic partition for a pair of surfaces. However, in a few cases, master-slave interactions are preferred. These cases consist of (1) interaction between an analytic surface and a deformable body, where the analytic body should be the master surface; and (2) contact between shells and solids,
where the solid should be the master surface.

### 7.15.3 Tolerances

\[
\begin{align*}
\text{NORMAL TOLERANCE} &= \text{<real>}\text{norm}_\text{tol} \\
\text{TANGENTIAL TOLERANCE} &= \text{<real>}\text{tang}_\text{tol} \\
\text{OVERLAP NORMAL TOLERANCE} &= \text{<real>}\text{over}_\text{norm}_\text{tol} \\
\text{OVERLAP TANGENTIAL TOLERANCE} &= \text{<real>}\text{over}_\text{tang}_\text{tol}
\end{align*}
\]

You can set tolerances for the interaction for a specific contact surface pair or for self-contact of a surface by using the above tolerance-related command lines in an `INTERACTION` command block. See Section 7.12.2 on search tolerances and Section 7.5 on overlap tolerances for a complete discussion of tolerances for contact.

### 7.15.4 Friction Model

\[
\text{FRICITION MODEL} = \text{<string>}\text{friction}_\text{model}_\text{name}|\text{FRICTIONLESS}
\]

You can set the friction model for the interaction for a specific contact surface pair or for self-contact of a surface by using the above command line in an `INTERACTION` command block. See Section 7.14.3 for a discussion of this command line.

### 7.15.5 Automatic Kinematic Partition

\[
\text{AUTOMATIC KINEMATIC PARTITION}
\]

You can turn on (or off) automatic kinematic partitioning for a specific contact surface pair by using the above command line in an `INTERACTION` command block. See Section 7.14.4 for a discussion of automatic kinematic partitioning.

### 7.15.6 Interaction Behavior

\[
\begin{align*}
\text{INTERACTION BEHAVIOR} &= \text{<string>}\text{SLIDING}| \\
\text{INFINITESIMAL}_\text{SLIDING}|\text{NO}_\text{INTERACTION}(\text{SLIDING})
\end{align*}
\]

You can set the search behavior for a specific contact surface pair or for self-contact of a surface by using the above command line in an `INTERACTION` command block. See Section 7.14.5 for a discussion of this command line.

A particular use of this command line in this particular command block is to set the interaction behavior to `NO_INTERACTION`. This deactivates enforcement between the surfaces specified in the `INTERACTION` command block.
7.16 Examples

This section has several example problems. We present the geometric configuration for the problems and the appropriate command lines to describe contact for the problems.

7.16.1 Example 1

Our first example problem has two blocks that come into contact due to initial velocity conditions. Block 1 has an initial velocity equal to $v_1$, and block 2 has an initial velocity equal to $v_2$. The geometric configuration for this problem is shown in Figure 7.6.

![Figure 7.6: Problem with two blocks coming into contact.](image)

The simplest input for this problem will be named EXAMPLE1 and is shown as follows:

```plaintext
BEGIN CONTACT DEFINITION EXAMPLE1
  # define contact surfaces
  SKIN ALL BLOCKS = ON

  # set interactions
  BEGIN INTERACTION DEFAULTS
    GENERAL CONTACT = ON
  END INTERACTION DEFAULTS
END
```

In our example, the `SKIN ALL BLOCKS` command line with its parameter set to ON will create a surface named `surface_1` (from the skinning of block_1) and a surface named `surface_2` (from the skinning of block_2).

All the normal and tangential tolerances will be set automatically in the above example. Frictionless contact is assumed. The kinematic partition factor defaults to 0.5 for both surfaces, `surface_1` and `surface_2`.

If you omitted the `INTERACTION DEFAULTS` command block with `GENERAL CONTACT` set to ON, then contact enforcement would not take place.
Now, let us consider the same problem (two blocks coming into contact) in which the contact definition for the problem is not defined simply by using all the default settings. The input for this variation of our two-block problem will be named EXAMPLE1A and is shown as follows:

```
BEGIN CONTACT DEFINITION EXAMPLE1A

    # define contact surfaces
    SKIN ALL BLOCKS = ON

    # friction model
    BEGIN CONSTANT FRICTION MODEL ROUGH
        FRICTION COEFFICIENT = 0.5
    END CONSTANT FRICTION MODEL ROUGH

    # search options
    BEGIN SEARCH OPTIONS
        GLOBAL SEARCH INCREMENT = 10
        NORMAL TOLERANCE = 1.0E-3
        TANGENTIAL TOLERANCE = 1.0E-3
    END SEARCH OPTIONS

    # set interactions
    BEGIN INTERACTION DEFAULTS
        FRICTION MODEL = ROUGH
        GENERAL CONTACT = ON
    END INTERACTION DEFAULTS

END
```

As is the case of the EXAMPLE1 command block, the SKIN ALL BLOCKS command line with its parameter set to ON will create a surface named surface_1 (from the skinning of block_1) and a surface named surface_2 (from the skinning of block_2).

For EXAMPLE1A, we want to have frictional contact between the two blocks. For the frictional contact, we define a constant friction model with a CONSTANT FRICTION MODEL command block. We name this model ROUGH.

The SEARCH OPTIONS command block sets the interval between global searches to 10; the default value is 5. Also, in this command block, we have set values for the normal and tangential tolerances. The option to compute the search tolerance automatically has been left on. The larger of the two values—an automatically computed tolerance or the user-specified tolerance—will be selected as the search tolerance during the search phase.

In the INTERACTION DEFAULTS command block, we select the friction model ROUGH on the FRICTION MODEL command line. As in the case of the EXAMPLE1 command block, if you omitted the INTERACTION DEFAULTS command block with GENERAL CONTACT set to ON, contact enforcement would not take place.
7.16.2 Example 2

Our second example problem has three blocks that come into contact due to initial velocity conditions. Block 1 has an initial velocity equal to $v_1$, and block 3 has an initial velocity equal to $v_3$. The geometric configuration for this problem is shown in Figure 7.7.

![Figure 7.7: Problem with three blocks coming into contact.](image)

The input for this three-block problem will be named `EXAMPLE2` and is shown as follows:

```
BEGIN CONTACT DEFINITION EXAMPLE2

    # define contact surfaces
    CONTACT SURFACE surface_1 CONTAINS block_1
    CONTACT SURFACE surface_2 CONTAINS block_2
    CONTACT SURFACE surf_3 CONTAINS surface_3

    # friction model
    BEGIN CONSTANT FRICTION MODEL ROUGH
        FRICTION COEFFICIENT = 0.5
    END CONSTANT FRICTION MODEL ROUGH

    # search options
    BEGIN SEARCH OPTIONS
        GLOBAL SEARCH INCREMENT = 10
        NORMAL TOLERANCE = 1.0E-3
        TANGENTIAL TOLERANCE = 1.0E-3
    END SEARCH OPTIONS

    # set interactions
    BEGIN INTERACTION DEFAULTS
        FRICTION MODEL = ROUGH
        GENERAL CONTACT = ON
```
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SELF CONTACT = ON
END INTERACTION DEFAULTS

# set specific interaction
BEGIN INTERACTION S2TOS3
    SURFACES = surface_2 surf_3
    KINEMATIC PARTITION = 0.4
    NORMAL TOLERANCE = 0.5E-3
    TANGENTIAL TOLERANCE = 0.5E-3
    FRICTION MODEL = FRICTIONLESS
END INTERACTION S2TOS3
END

For the EXAMPLE2 command block, we have defined three surfaces. The first surface, surface_1, is obtained by skinning block_1. The second surface, surface_2 is obtained by skinning block_2. The third surface, surf_3, is the user-defined surface surface_3. The user-defined surface, surface_3, can contain a subset of the external element faces that define block_3 or all the external element faces that define block_3.

The SEARCH OPTIONS command block sets the interval between global searches to 10; the default value is 5. Also, in this command block, we have set values for the normal and tangential tolerances. The option to compute the search tolerance automatically has been left on. The larger of the two values—an automatically computed tolerance or the user-specified tolerance—will be selected as the search tolerance during the search phase.

In the INTERACTION DEFAULTS command block, we select the friction model ROUGH on the FRICTION MODEL command line. Both GENERAL CONTACT and SELF CONTACT are set to ON in the EXAMPLE2 command block. For this problem, block_2 can undergo self-contact. Setting GENERAL CONTACT to ON will enforce contact between surface_1 and surface_2, surface_2 and surf_3, and surface_1 and surf_3. Setting SELF CONTACT to ON will enforce self-contact for all three of the surfaces.

For this particular example, we want to override some of the Presto default values for surface interaction and some of the default values for surface interaction set by the INTERACTION DEFAULTS command block for the interaction between surface_2 and surf_3. To override default values, we use an INTERACTION command block and indicate that it applies to surface_2 and surf_3 with a SURFACES command line. We override the Presto default for the kinematic partition factor by using a KINEMATIC PARTITION command line with the kinematic partition parameter set to a value of 0.4. We override the normal and tangential tolerances and the friction model set in the INTERACTION command block. The normal and tangential tolerances for interaction between surface_2 and surf_3 is set to 0.5E-3 rather than the global value of 1.0E-3. The friction model for interaction between surface_2 and surf_3 is set to FRICTIONLESS rather than the default value of ROUGH.
7.17 Dash Contact

CONTACT FORMULATION TYPE = ACME|DASH\(\text{ACME}\)

Dash is an alternative contact algorithm that is a replacement for the ACME explicit dynamics contact algorithm. The Dash algorithm is selected with the contact formulation type command. Generally any existing ACME contact command block may be converted to a Dash command block simply by using this one command. However, Dash will ignore some ACME options so is only applicable on a subset of problems that ACME can run.

### 7.17.1 How Dash is Different from ACME

Dash is a facet based enforcement algorithm. Dash attempts to compute the total volume of overlap between two facet sets and remove the overlap. In contrast ACME only removes the gap between nodes and faces. Dash uses a reduced order area integration scheme for calculation and removal of volumetric overlaps.

In some case Dash is more robust than ACME and can more accurately solve certain classes of problems. One type of problem where Dash often works better than ACME are high loading rates and stiffening materials. ACME contact enforcement tends to aggravate hourglass modes when used on these types of problems. Additionally problems where ACME tolerancing issues, multiple interaction issues, or topology restrictions cause ACME to perform poorly may be run more robustly with Dash.

However, Dash results for frictional behavior is generally less accurate than is ACME. Dash is less able to exactly capture the transition from sticking to slipping behavior and other such frictional details than is ACME.

Dash is designed to work correctly for a wide variety of problems with minimal user tweaking. It is generally recommended that Dash be used with a minimal set of inputs, for example `skin all blocks`, `self and/or general contact = on`, and interaction friction models. Dash has no tolerances, kinematic partitions, or any other such inputs.

Dash uses an iterative penalty based enforcement scheme. Dash enforcement explicitly balances Momentum by always applying equal and opposite forces.

### 7.17.2 Current Dash Usage Guidelines

Use Dash for remeshing problems. ACME does not perform well on changing topologies. Dash may also be useful for problems with element death. ACME often must artificially kill a large number of additional elements other than those which have reached a user defined death criteria. ACME requires these additional element removals in order to work around certain ACME surface topology restrictions. Dash has no topology restrictions so does not need to kill any extra elements to maintain a valid contact topology.
Dash is often significantly faster than ACME, particularly on parallel problems. Speedups from 1.5 to 4 times have been observed on a wide range of problems when using Dash as compared to ACME.

The following ACME capabilities are not currently supported by Dash:

- Analytic Surfaces
- Point (node set or particle) Contact
- Shell Contact
- 8 and 10 node tetrahedron contact
- Complex friction models (anything other than frictionless, constant friction, glued, and tied tied contact at a distance. Dash assumes all contact occurs at a nominal gap of zero. Tolerances specified in the input deck are currently ignored.
- Rigid body contact
- Contact variable output

Additionally avoid using side set contact with Dash and prefer block skinning. Dash contains ray tracing algorithms to determine if certain contact points are inside or outside of bodies. If the surfaces Dash is using do not define fully enclosed bodies Dash may become confused and think a point inside the body is actually outside the body or vice versa.

Dash accepts the same surface definitions as does ACME. Dash also uses identical syntax for interaction definition. The relevant contact block options for Dash are:

```plaintext
CONTACT SURFACE <name> CONTAINS <surface_name>
CONTACT SURFACE <name> CONTAINS <block_name>

BEGIN INTERACTION DEFAULTS
  GENERAL CONTACT = ON|OFF (OFF)
  SELF CONTACT = ON|OFF (OFF)
  DEFAULT FRICTION MODEL = <string>(default_frictionless)
END

BEGIN FRICTIONLESS MODEL <name>
END FRICTIONLESS MODEL

BEGIN CONSTANT FRICTION MODEL <name>
  FRICTION COEFFICIENT = <real>coeff
END CONSTANT FRICTION MODEL

BEGIN TIED FRICTION MODEL <name>
END TIED FRICTION MODEL
```
BEGIN GLUED FRICTION MODEL <name>
END GLUED FRICTION MODEL

BEGIN INTERACTION
  SURFACES = <name> <name>
  MASTER = <name>
  SLAVE = <name>
  FRICTION MODEL = <name>
END INTERACTION

BEGIN ENFORCEMENT OPTIONS
  MOMENTUM BALANCE ITERATIONS = <integer>(5)
  NUM GEOMETRY UPDATE ITERATIONS = <integer>(1)
END

BEGIN OVERLAP REMOVAL
END OVERLAP REMOVAL

BEGIN DASH OPTIONS
  SCALE FACTOR = <real>factor(1.0)
  DICE FACES = <string>ON|OFF (ON)
  INTERACTION DEFINITION SCHEME = <string>DASH_DEFAULT|EXPLICIT(DASH_DEFAULT)
  SEARCH LENGTH SCALING = <real>factor(0.1)
END

BEGIN DEBUG
  OUTPUT LEVEL = <integer>(0)
END DEBUG

All contact definition block commands not listed above are ignored by Dash. This includes contact tolerances, kinematic partitions, ACME performance options, etc. The contact surface definition, interaction definition, and friction model specification commands work identically to their ACME counterparts. The four supported friction models also behave identically to the ACME versions of those friction models.

The **MOMENTUM BALANCE ITERATIONS** command controls how many iterative enforcement passes Dash will perform. For Dash these are not really momentum balance iterations as Dash explicitly balances momentum at every iteration. Increasing the number of momentum balance iterations will increase result accuracy, minimizing overlap and better conserving energy terms.

**NUM GEOMETRY UPDATE ITERATIONS** is unique to Dash. This command allows the contact search geometry to be updated multiple times per search step. Larger values for this command yield better enforcement, but at significantly increased cost.

The **DASH OPTIONS** command block contains a few options unique to Dash. Generally Dash is designed to run accurately with as few knobs as possible, however a few options do exist.
The **SCALE FACTOR** command defines the final scaling factor to apply to contact forces. This is mostly a developer option to help debug certain contact pathologies.

The **DICE FACES** command tells Dash to use a face dicing scheme to enforce removal of volumetric overlap. By default Dash intersects all contact faces with themselves and keeps only the portions of faces found inside of another body for contact. Turning off face dicing turns faces into single points. Without dicing a face is a candidate for contact only if the centroid of the face is inside of another body.

With face dicing on, full volumetric enforcement is obtained (with enough enforcement iterations.) With face dicing off, volume overlap enforcement is not guaranteed, however, the algorithm may run significantly faster. Face dicing is vital for correct enforcement of corner contacts, but if all contact surfaces are relatively smooth turning off face dicing may yield substantial speed benefits with little accuracy loss.

The **INTERACTION DEFINITION SCHEME** command controls how contact interactions are defined. By default all Dash interactions are one sided. As the full volume of overlap is removed there is really no concept of master face or slave face. By default Dash picks an optimal enforcement order for each interaction pair based on face size. However, the ability exists to explicitly use the potentially symmetric interactions defined in the input deck by supplying the EXPLICIT option to this command. This may allow better enforcement in some circumstances, particularly tied contact.

The **SEARCH LENGTH SCALING** command defines how far into a body Dash will search for potentially interacting faces. The search tolerance is a multiplier on the face characteristic length. If faces move farther than (SEARCH LENGTH SCALING) times (FACE CHARACTERISTIC LENGTH) in single time step contact could be lost. Thus extremely high velocity contacts may require use of higher values of search length scaling. Note, the default values used should be sufficient for impact speeds bellow the material sound speed.
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7.18 References


Chapter 8

Output

Presto produces a variety of output. This chapter discusses how to control the four major types of output: results output, history output, heartbeat output, and restart output. Results output lets the user select some set of variables (registered, user-defined, or some combination thereof). If the user selects a nodal variable such as displacement for results output, the displacements for all the nodes in a model will be output to a results file. If the user selects an element variable such as rotated stress for results output, the rotated stress for all elements in the model that calculate this quantity (rotated stress) will be output. The history output option lets the user select a very specific set of information for output. For example, if you know that the displacement at a particular node is critical, then you can select only the displacement at that particular node as history output. The heartbeat output is similar to the history output except that the output is written to a text file instead of to a binary (exodusII [1]) file. The restart output is written so that any calculation can be halted at some arbitrary analysis time and then restarted at this time. The user has no control over what is written to the restart file. When a restart file is written, it must be a complete state description of the calculations at some given time. A restart file contains a great deal of information and is typically much larger than a results file. You need to carefully limit how often a restart file is written.

Section 8.1 describes the results output. Included in the results output is a description of commands for user-defined output (Section 8.1.2). User-defined output lets the user postprocess analysis results as the code is running to produce a reduced set of output information. Section 8.2 describes the history output, Section 8.3 describes the heartbeat output, and Section 8.4 describes the restart output. All four types of output (results, history, heartbeat, and restart) can be synchronized for analyses with multiple regions. This scheduling functionality is discussed in Section 8.5. In Section 8.6, there is a list of key registered variables.

Unless otherwise noted, the command blocks and command lines discussed in Chapter 8 appear in the region scope.
8.1 Results Output

The results output capability lets you select some set of variables that will be written to a file at various intervals. As previously indicated, all the values for each selected variable will be written to the results file. (The interval at which information is written can be changed throughout the analysis time.) The name of the results file is set in the RESULTS OUTPUT command block.
8.1. Exodus Results Output File

BEGIN RESULTS OUTPUT <string>results_name
   DATABASE NAME = <string>results_file_name
   DATABASE TYPE = <string>database_type(exodusII)
   OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
               (ON|TRUE|YES)
   TITLE <string>user_title
   NODE VARIABLES = <string>variable_name
                     [AS <string>dbase_variable_name] ...
                     <string>variable_name [AS
                     <string>dbase_variable_name]
     | NODAL VARIABLES = <string>variable_name
                     [AS <string>dbase_variable_name] ...
                     <string>variable_name [AS
                     <string>dbase_variable_name]
   NODESET VARIABLES = <string>variable_name
                     [AS <string>dbase_variable_name] ...
                     <string>variable_name [AS
                     <string>dbase_variable_name]
     | NODESET VARIABLES = <string>variable_name
                     [AS <string>dbase_variable_name]
                     INCLUDE|ON|EXCLUDE <string list>nodelist_names
                     ... <string>variable_name
                     [AS <string>dbase_variable_name] INCLUDE|ON|EXCLUDE
                     <string list>nodelist_names
   FACE VARIABLES = <string>variable_name
                     [AS <string>dbase_variable_name] ...
                     <string>variable_name [AS
                     <string>dbase_variable_name]
     | FACE VARIABLES = <string>variable_name
                     [AS <string>dbase_variable_name]
                     INCLUDE|ON|EXCLUDE <string list>surface_names
                     ... <string>variable_name
                     [AS <string>dbase_variable_name] INCLUDE|ON|EXCLUDE
                     <string list>surface_names
   ELEMENT VARIABLES = <string>variable_name
                     [AS <string>dbase_variable_name] ...
                     <string>variable_name [AS
                     <string>dbase_variable_name]
     | ELEMENT VARIABLES = <string>variable_name
                     [AS <string>dbase_variable_name]
                     INCLUDE|ON|EXCLUDE <string list>block_names
                     ... <string>variable_name
                     [AS dbase_variable_name] INCLUDE|ON|EXCLUDE
                     <string list>block_names
   OUTPUT MESH = EXPOSED_SURFACE|BLOCK_SURFACE
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COMPONENT SEPARATOR CHARACTER = <string>character|NONE
GLOBAL VARIABLES = <string>variable_name
    [AS <string>dbase_variable_name] ...
    <string>variable_name [AS
    <string>dbase_variable_name]
START TIME = <real>output_start_time
TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
AT TIME <real>time_begin INCREMENT =
    <real>time_increment_dt
ADDITIONAL TIMES = <real>output_time1
    <real>output_time2 ...
AT STEP <integer>step_begin INCREMENT =
    <integer>step_increment
ADDITIONAL STEPS = <integer>output_step1
    <integer>output_step2 ...
TERMINATION TIME = <real>termination_time_value
USE OUTPUT SCHEDULER <string>scheduler name
OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
    SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
    SIGILL|SIGILL|SIGSEGV
END [RESULTS OUTPUT <string>results_name]

You can specify a results file, the results to be included in this file, and the frequency at which results are written by using a RESULTS OUTPUT command block. The command block appears inside the region scope.

More than one results file can be specified for an analysis. Thus for each results file, there will be one RESULTS OUTPUT command block. The command block begins with:

    BEGIN RESULTS OUTPUT <string>results_name

and is terminated with:

    END [RESULTS OUTPUT <string>results_name]

where results_name is a user-selected name for the command block. Nested within the RESULTS OUTPUT command block are a set of command lines, as shown in the block summary given above. The first two command lines listed (DATABASE NAME and DATABASE TYPE) give pertinent information about the results file. The command line

    DATABASE NAME = <string>results_file_name

gives the name of the results file with the string results_file_name. If the results file is to appear in the current directory and is named job.e, this command line would appear as:

    DATABASE NAME = job.e

If the results file is to be created in some other directory, the command line would have to show the path to that directory.

If the results file does not use the Exodus II format [1], you must specify the format for the results file using the command line:
DATABASE TYPE = <string>database_type(exodusII)

Currently, both the Exodus II database and the XDMF database [2] are supported in Presto and Adagio. Exodus II is more commonly used than XDMF. Other options may be added in the future.

The OVERWRITE command line can be used to prevent the overwriting of existing results files.

OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO

The OVERWRITE command line allows only a single value. If you set the value to FALSE, NO, or OFF, the code will terminate before existing results files can be overwritten. If you set the value to TRUE, YES, or ON, then existing results files can be overwritten (the default status). Suppose, for example, that we have an existing results file named job21.e. Suppose also that we have an input file with a RESULTS OUTPUT command block that contains the OVERWRITE command line set to ON and the DATABASE NAME command line set to:

DATABASE NAME = job21.e

If you run the code under these conditions, the existing results file job21.e will be overwritten.

Whether or not results files are overwritten is also impacted by the use of the automatic read and write option for restart files described in Section 8.4.1.1. If you use the automatic read and write option for restart files, the results files, like the restart files, are automatically managed. The automatic read and write option in restart adds extensions to file names and prevents the overwriting of any existing restart or results files. For the case of a user-controlled read and write of restart files (Section 8.4.1.2) or of no restart, however, the OVERWRITE command line is useful for preventing the overwriting of results files.

You may add a title to the results file by using the TITLE command line. Whatever you specify for the user_title will be written to the results file. Some of the programs that process the results file (such as various SEACAS programs [3]) can read and display this information.

The other command lines that appear in the RESULTS OUTPUT command block determine the type and frequency of information that is output. Descriptions of these command lines follow in Section 8.1.1.1 through Section 8.1.1.16.

8.1.1.1 Output Nodal Variables

NODE VARIABLES = <string>variable_name
| [AS <string>dbase_variable_name] ...
<variable_name> [AS <string>dbase_variable_name]
| NODAL VARIABLES = <string>variable_name
| [AS <string>dbase_variable_name] ...
<variable_name> [AS <string>dbase_variable_name]

Any nodal variable in Presto can be selected for output in the results file by using a command line in one of the two forms shown above. The only difference between the two forms is the use of
The string variable_name is the name of the nodal variable to output. The string variable_name can be either a registered variable listed in Section 8.6 or a user-defined variable (see Section 8.1.2 and Section 9.2.4).

For the above two command lines, any nodal variable requested for output is output for all nodes.

It is possible to specify an alias for any of the nodal variables by using the AS specification. Suppose, for example, you wanted to output the external forces in Presto, which are registered as force_external, with the alias f_ext. You would then enter the command line:

```
NODE VARIABLES = force_external AS f_ext
```

In this example, the external force is a vector quantity. For a vector quantity at a node, suffixes are appended to the variable name (or alias name) to denote each vector component. The results database would have three variable names associated with the external force: f_ext_x, f_ext_y, and f_ext_z. Consult with Table 8.4 for a list of component identifiers for vectors. You can change the component separator, an underscore in this example, by using the COMPONENT SEPARATOR CHARACTER command line (see Section 8.1.1.6).

The NODE VARIABLES command line can be used an arbitrary number of times within a RESULTS OUTPUT command block. It is also possible to specify more than one nodal variable for output on a command line, as indicated by the ellipsis in the command line format. In the following example, two nodal variables are specified for output. Note that the internal forces are registered as force_internal.

```
NODE VARIABLES = force_external force_internal
```

Aliases can be specified for each of the variables in a single command line. Thus, if you wanted to output the alias f_ext for external forces and also wanted to output the alias f_int for internal forces, you would enter the command line:

```
NODE VARIABLES = force_external AS f_ext
force_internal AS f_int
```

The specification of an alias is always optional.

### 8.1.1.2 Output Node Set Variables

```
NODESET VARIABLES = <string>variable_name
| AS <string>dbase_variable_name | ...

<string>variable_name [AS <string>dbase_variable_name]
| NODESET VARIABLES = <string>variable_name
| AS <string>dbase_variable_name
| INCLUDE|ON|EXCLUDE <string list>nodelist_names
...

<string>variable_name
| AS <string>dbase_variable_name | INCLUDE|ON|EXCLUDE <string list>nodelist_names
```
A nodal variable may be registered only on a subset of the total set of nodes defining a model. A nodal variable that is registered only on some subset of nodes is referred to as a node set variable. The NODESET VARIABLES command line lets you specify a node set variable for output to the results file.

There are two forms of the NODESET VARIABLES command line. Either form will let you output a node set variable.

The first form of the command line is as follows:

```
NODESET VARIABLES = <string>variable_name
                   [AS <string>dbase_variable_name] ...
                   <string>variable_name [AS
                   <string>dbase_variable_name]
```

Here, the string variable_name is a node set variable associated with one or more node sets. In this form, the node set variable is output for all node sets associated with that node set variable.

It is possible to specify an alias in the results file for any of the node set variables by using the AS specification. Suppose, for example, you wanted to output a node set variable registered as force_nsetype with the alias fnsetype. You would then enter the command line:

```
NODESET VARIABLES = force_nsetype AS fnsetype
```

The NODESET VARIABLES command line can be used an arbitrary number of times within a RESULTS OUTPUT command block. It is also possible to specify more than one node set variable for output on a command line, as indicated by the ellipsis in the command line format. In the following example, two node set variables are specified for output. Here, the second node set variable is registered as force_nsetype2.

```
NODESET VARIABLES = force_nsetype force_nsetype2
```

Aliases can be specified for each of the variables in a single command line. Thus, if you wanted to output the alias fnsetype for node set variable force_nsetype and also wanted to output the alias fnsetype2 for node set variable force_nsetype2, you would enter the command line:

```
NODESET VARIABLES = force_nsetype AS fnsetype
                   force_nsetype2 AS fnsetype2
```

The specification of an alias is always optional.

The second form of the command line is as follows:

```
NODESET VARIABLES = <string>variable_name
                   [AS <string>dbase_variable_name]
                   INCLUDE|ON|EXCLUDE <string list>nodelist_names
                   ... <string>variable_name
                   [AS <string>dbase_variable_name] INCLUDE|ON|EXCLUDE
                   <string list>nodelist_names
```

This form of the NODESET VARIABLES command line is similar to the first, except that the user can control which node sets are used for output. The user can include a specific list of node sets
for output by using the INCLUDE option or the ON option. (The key word INCLUDE is synonymous with the key word ON.) Alternatively, the user can exclude a specific list of node sets for output by using the EXCLUDE option.

Suppose that the node set variable force_nsetype from the above example has been registered for nodelist_10, nodelist_11, nodelist_20, and nodelist_21. If we only want to output the node set variable for node sets nodelist_10, nodelist_11, and nodelist_21, then we could specify the NODESET VARIABLES command line as follows:

\[
\text{NODESET VARIABLES} = \text{force_nsetype AS fnsetype} \\
\quad \text{INCLUDE} \ nodelist_10, \ nodelist_11, \ 
\quad \text{nodelist}_21
\]

(In the above command line, the keyword ON could be substituted for INCLUDE.) Alternatively, we could use the command line:

\[
\text{NODESET VARIABLES} = \text{force_nsetype AS fnsetype} \\
\quad \text{EXCLUDE} \ nodelist_20
\]

In the above command lines, an alias for a node set can be substituted for a node set identifier. For example, if center_case is an alias for nodelist_10, then the string center_case could be substituted for nodelist_10 in the above command lines. Because a node set identifier is a mesh entity, the alias for the node set identifier would be defined via an ALIAS command line in a FINITE ELEMENT MODEL command block.

Note that the list of identifiers uses a comma to separate one node set identifier from the next node set identifier.

### 8.1.1.3 Output Face Variables

\[
\text{FACE VARIABLES} = \langle \text{string}\rangle\text{variable_name} \\
\quad [\text{AS} \langle \text{string}\rangle\text{dbase_variable_name}] \ldots \\
\langle \text{string}\rangle\text{variable_name} [\text{AS} \langle \text{string}\rangle\text{dbase_variable_name}] \\
| \text{FACE VARIABLES} = \langle \text{string}\rangle\text{variable_name} \\
\quad [\text{AS} \langle \text{string}\rangle\text{dbase_variable_name}] \\
\quad \text{INCLUDE|ON|EXCLUDE} \langle \text{string list}\rangle\text{surface_names} \\
\quad \ldots \langle \text{string}\rangle\text{variable_name} \\
\quad [\text{AS} \langle \text{string}\rangle\text{dbase_variable_name}] \text{INCLUDE|ON|EXCLUDE} \langle \text{string list}\rangle\text{surface_names}
\]

A variable may be registered on some set of faces that constitute a surface. A variable registered on a set of faces is referred to as a face variable. The FACE VARIABLES command line lets you specify a face variable for output to the results file.

There are two forms of the FACE VARIABLE command line. Either form will let you output a face variable.

The first form of the command line is as follows:
FACE VARIABLES = <string>variable_name
    [AS <string>dbase_variable_name] ...
    <string>variable_name [AS
    <string>dbase_variable_name]

Here, the string variable_name is a face variable associated with one or more surfaces. In this form, the face variable is output for all surfaces associated with that face variable.

It is possible to specify an alias in the results file for any face variable by using the AS specification. Suppose, for example, you wanted to output a face variable registered as pressure_face with the alias pressuref. You would then enter the command line:

    FACE VARIABLES = pressure_face AS pressuref

The FACE VARIABLES command line can be used an arbitrary number of times within a RESULTS OUTPUT command block. It is also possible to specify more than one face variable for output on a command line, as indicated by the ellipsis in the command line format. In the following example, two face variables are specified for output. Here, the second face variable is registered as scalar_face2.

    FACE VARIABLES = pressure_face scalar_face2

Aliases can be specified for each of the variables in a single command line. Thus, if you wanted to output the alias pressuref for face variable pressure_face and also wanted to output the alias scalarf2 for face variable scalar_face2, you would enter the command line:

    FACE VARIABLES = pressure_face AS pressuref
                   scalar_face2 AS scalarf2

The specification of an alias is always optional.

The second form of the command line is as follows:

    FACE VARIABLES = <string>variable_name
                    [AS <string>dbase_variable_name]
                    INCLUDE|ON|EXCLUDE <string list>surface_names
                    ... <string>variable_name
                    [AS <string>dbase_variable_name] INCLUDE|ON|EXCLUDE
                    <string list>surface_names

This form of the FACE VARIABLES command line is similar to the first, except that the user can control which surfaces are used for output. The user can include a specific list of surfaces for output by using the INCLUDE option or the ON option. (The key word INCLUDE is synonymous with the keyword ON.) Alternatively, the user can exclude a specific list of surfaces for output by using the EXCLUDE option.

Suppose that the face variable pressure_face from the above example has been registered for surface_10, surface_11, surface_20, and surface_21. If we only want to output the face variable for surface_10, surface_11, and surface_21, then we could specify the FACE VARIABLES command line as follows:
FACE VARIABLES = pressure_face AS pressuref
   INCLUDE surface_10, surface_11,
          surface_21

(In the above command line, the keyword ON could be substituted for INCLUDE.) Alternatively, we
could use the command line:

FACE VARIABLES = pressure_face AS pressuref
   EXCLUDE surface_20

In the above command lines, an alias for a surface can be substituted for a surface identifier.
For example, if center_case is an alias for surface_10, then the string center_case could
be substituted for surface_10 in the above command lines. Because a surface identifier is a
mesh entity, the alias for the surface identifier would be defined via an ALIAS command line in a
FINITE ELEMENT MODEL command block.

Note that the list of identifiers uses a comma to separate one surface identifier from the next surface
identifier.

8.1.1.4 Output Element Variables

ELEMENT VARIABLES = <string>variable_name
   [AS <string>dbase_variable_name] ...
   <string>variable_name [AS
   <string>dbase_variable_name]
| ELEMENT VARIABLES = <string>variable_name
   [AS <string>dbase_variable_name]
   INCLUDE|ON|EXCLUDE <string list>block_names
   ... <string>variable_name
   [AS dbase_variable_name] INCLUDE|ON|EXCLUDE
   <string list>block_names

Any element variable in Presto can be selected for output in the results file by using the ELEMENT
VARIABLES command line.

There are two forms of the ELEMENT VARIABLES command line. Either form will let you output
an element variable.

The first form of the command line is as follows:

ELEMENT VARIABLES = <string>variable_name
   [AS <string>dbase_variable_name] ...
   <string>variable_name [AS
   <string>dbase_variable_name]

Here, the string variable_name is the name of the element variable to output. The string
variable_name can be a registered variable listed in Section 8.6, a user-defined variable (see
Section 8.1.2 and Section 9.2.4), or a derived output quantity. The derived output option is discussed in detail in the latter portion of this discussion of the ELEMENT VARIABLES command line.

In the first form of the ELEMENT VARIABLES command line, the element variable is output for all element blocks that have the element variable as a registered variable. For example, all the solid elements have rotated_stress as a registered variable. If you had a mesh consisting of hexahedral and tetrahedral elements and requested output of the element variable rotated_stress, then rotated_stress would be output for all element blocks consisting of hexahedral and tetrahedral elements.

It is possible to specify an alias for any of the element variables by using the AS specification. Suppose, for example, you wanted to output the stress in Presto, which is registered as rotated_stress, with the alias stress. You would then enter the command line:

```
ELEMENT VARIABLES = rotated_stress AS stress
```

In this example, stress is a symmetric tensor quantity. For a symmetric tensor quantity, suffixes are appended to the variable name (or alias name) to denote each symmetric tensor component. The results database would have six variable names associated with the stress: stress_xx, stress_yy, stress_zz, stress_xy, stress_xz, and stress_yz. Consult with Table 8.4 for a list of component identifiers for symmetric and full tensors. You can change the tensor component separator, an underscore in this example, by using the COMPONENT SEPARATOR CHARACTER command line (see Section 8.1.1.6).

The ELEMENT VARIABLES command line can be used an arbitrary number of times within a RESULTS OUTPUT command block. It is also possible to specify more than one element variable for output on a command line, as indicated by the ellipsis in the command line format. In the following example, two element variables are specified for output. Here, the second element variable is registered as stretch.

```
ELEMENT VARIABLES = rotated_stress stretch
```

Aliases can be specified for each of the variables in a single command line. Thus, if you wanted to output the alias stress for element variable rotated_stress and also wanted to output the alias strch for face variable stretch, you would enter the command line:

```
ELEMENT VARIABLES = rotated_stress AS stress
                     stretch AS strch
```

The specification of an alias is always optional.

The second form of the command line is as follows:

```
ELEMENT VARIABLES = <string>variable_name
                     [AS <string>dbase_variable_name]
                     INCLUDE|ON|EXCLUDE <string list>block_names
                     ... <string>variable_name
                     [AS dbase_variable_name] INCLUDE|ON|EXCLUDE
                     <string list>block_names
```
This form of the `ELEMENT VARIABLES` command line is similar to the first, except that the user can control which element blocks are used for output. The user can include a specific list of element blocks for output by using the `INCLUDE` option or the `ON` option. (The key word `INCLUDE` is synonymous with the key word `ON`.) Alternatively, the user can exclude a specific list of element blocks for output by using the `EXCLUDE` option.

Suppose that the element variable `rotated_stress` from the above example exists for element blocks `block_10`, `block_11`, `block_20`, and `block_21`. If we only want to output the element variable for `block_10`, `block_11`, and `block_21`, then we could specify the `ELEMENT VARIABLES` command line as follows:

```
ELEMENT VARIABLES = rotated_stress AS stress
    INCLUDE block_10, block_11, block_21
```

(In the above command line, the keyword `ON` could be substituted for `INCLUDE`.) Alternatively, we could use the command line:

```
ELEMENT VARIABLES = rotated_stress AS stress
    EXCLUDE block_20
```

In the above command lines, an alias for an element block can be substituted for an element block identifier. For example, if `center_case` is an alias for `block_10`, then the string `center_case` could be substituted for `block_10` in the above command lines. Because an element block identifier is a mesh entity, the alias for the element block identifier would be defined via an `ALIAS` command line in a `FINITE ELEMENT MODEL` command block.

Note that the list of identifiers uses a comma to separate one element block identifier from the next element block identifier.

As mentioned previously, you can use the `ELEMENT VARIABLES` command line for the output of a derived quantity. Derived quantities are calculated for solid elements and for shell elements. A derived quantity is identified by supplying one of the available options listed in Table 8.1, Table 8.2, or Table 8.3 for the string `variable_name`. For example, you would use the following command to compute and output von Mises stress on all solid elements:

```
ELEMENT VARIABLES = von_mises
```

Table 8.1 gives the complete set of derived stresses for solid elements and for shell elements. For the shell elements, the derived quantities from the stress tensor are given at each of the integration points. For the shell elements, the derived quantities from the stress are given at each of the integration points. A suffix ranging from 1 to the number of integration points is attached to the derived quantity to indicate the corresponding integration point. The suffix is padded with leading zeros. If the number of integration points is less than 10, the suffix has the form `_i`, where `i` ranges from 1 to the number of integration points. If the number of integration points is greater than or equal to 10 and less than 100, the sequence of suffixes takes the form `_01, _02, _03,`
and so forth. Finally, if the number of integration points is greater than or equal to 100, the sequence of suffixes takes the form _001, _002, _003, and so forth. As an example, if the von Mises stress is requested for a shell element with 15 integration points, then the derived quantities von_mises_01, von_mises_02, ..., von_mises_15 are output for the shell element.

Table 8.1: Derived Stress Output for Elements

<table>
<thead>
<tr>
<th>Option</th>
<th>Option Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>von_mises</td>
<td>Von Mises stress norm.</td>
</tr>
<tr>
<td>hydrostatic_stress</td>
<td>One-third the trace of the stress sensor.</td>
</tr>
<tr>
<td>stress_invariant_1</td>
<td>Trace of the stress tensor.</td>
</tr>
<tr>
<td>stress_invariant_2</td>
<td>Second invariant of the stress tensor.</td>
</tr>
<tr>
<td>stress_invariant_3</td>
<td>Third invariant of the stress tensor.</td>
</tr>
<tr>
<td>max_principal_stress</td>
<td>Largest eigenvalue of the stress tensor.</td>
</tr>
<tr>
<td>intermediate_principal_stress</td>
<td>Middle eigenvalue of the stress tensor.</td>
</tr>
<tr>
<td>min_principal_stress</td>
<td>Smallest eigenvalue of the stress tensor.</td>
</tr>
<tr>
<td>max_shear_stress</td>
<td>Maximum shear stress from Mohr’s circle.</td>
</tr>
<tr>
<td>octahedral_shear_stress</td>
<td>Octahedral shear norm of the stress tensor.</td>
</tr>
</tbody>
</table>

Most solid elements use only one integration point. For solid elements with multiple integration points, the conventions used for multiple integration points in shells are also used for multiple integration points in solids.

In the above discussion concerning the format for output at multiple integration points, the underscore character preceding the integration point number can be replaced by another delimiter or the underscore character can be eliminated by use of the COMPONENT SEPARATOR CHARACTER command line (see Section 8.1.1.6).

Table 8.2 gives the complete set of quantities derived from the log strain for solid elements. (Solid elements generate log strain information, while shell elements generate integrated strain information.)
Table 8.2: Derived Log Strain Output for Solid Elements

<table>
<thead>
<tr>
<th>Option</th>
<th>Option Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>effective_log_strain</td>
<td>Effective log strain.</td>
</tr>
<tr>
<td>log_strain_invariant_1</td>
<td>Trace of the log strain tensor.</td>
</tr>
<tr>
<td>log_strain_invariant_2</td>
<td>Second invariant of the log strain tensor.</td>
</tr>
<tr>
<td>log_strain_invariant_3</td>
<td>Third invariant of the log strain tensor.</td>
</tr>
<tr>
<td>max_principal_log_strain</td>
<td>Largest eigenvalue of the log strain tensor.</td>
</tr>
<tr>
<td>intermediate_principal_log_strain</td>
<td>Middle eigenvalue of the log strain tensor.</td>
</tr>
<tr>
<td>min_principal_log_strain</td>
<td>Smallest eigenvalue of the log strain tensor.</td>
</tr>
<tr>
<td>max_shear_log_strain</td>
<td>Maximum shear log strain from Mohr’s circle.</td>
</tr>
<tr>
<td>octahedral_shear_log_strain</td>
<td>Octahedral strain norm of the log strain tensor.</td>
</tr>
</tbody>
</table>

Most solid elements use only one integration point. For solid elements with multiple integration points, the conventions used for multiple integration points in shells are also used for multiple integration points in solids.

Table 8.3 gives the complete set of quantities derived from the integrated strain for shell elements. (Solid elements generate log strain information, while shell elements generate integrated strain information.) For the shell elements, the derived quantities from the integrated strain are given at each of the integration points. A suffix ranging from 1 to the number of integration points is attached to the derived quantity to indicate the corresponding integration point. The suffix is padded with leading zeros. If the number of integration points is less than 10, the suffix has the form \(_i\), where \(i\) ranges from 1 to the number of integration points. If the number of integration points is greater than or equal to 10 and less than 100, the sequence of suffixes takes the form \(_01, _02, _03\), and so forth. Finally, if the number of integration points is greater than or equal to 100, the sequence of suffixes takes the form \(_001, _002, _003\), and so forth. As an example, if the effective strain is requested for a shell element with 15 integration points, then the derived quantities effective_strain_01, effective_strain_02, ..., effective_strain_15 are output for the shell element.

In the above discussion concerning the output format for multiple integration points for shells, the underscore character preceding the integration point number can be replaced by another delimiter, or the underscore character can be eliminated by use of the COMPONENT SEPARATOR CHARACTER command line (see Section 8.1.1.6).
Table 8.3: Derived Strain Output for Shell Elements

<table>
<thead>
<tr>
<th>Option</th>
<th>Option Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>effective_strain</td>
<td>Effective strain.</td>
</tr>
<tr>
<td>strain_invariant_1</td>
<td>Trace of the strain tensor.</td>
</tr>
<tr>
<td>strain_invariant_2</td>
<td>Second invariant of the strain tensor.</td>
</tr>
<tr>
<td>strain_invariant_3</td>
<td>Third invariant of the strain tensor.</td>
</tr>
<tr>
<td>max_principal_strain</td>
<td>Largest eigenvalue of the strain tensor.</td>
</tr>
<tr>
<td>intermediate_principal_strain</td>
<td>Middle eigenvalue of the strain tensor.</td>
</tr>
<tr>
<td>min_principal_strain</td>
<td>Smallest eigenvalue of the strain tensor.</td>
</tr>
<tr>
<td>max_shear_strain</td>
<td>Maximum shear strain from Mohr’s circle.</td>
</tr>
<tr>
<td>octahedral_shear_strain</td>
<td>Octahedral strain norm of the strain tensor.</td>
</tr>
</tbody>
</table>

8.1.1.5 Output Mesh Selection

```
OUTPUT MESH = EXPOSED_SURFACE|BLOCK_SURFACE
```

The OUTPUT MESH command provides a way to reduce the amount of data that is written to the results database. There are two options that can be selected:

**EXPOSED_SURFACE** Only output the element faces that make up the “skin” of the finite element model; no internal nodes or elements will be written to the results database. The element results variables will be applied to the skin faces. If the mesh is visualized without any cutting planes, the display should look the same as if the original full mesh were visualized; however, the amount of data written to the output file can be much less than is needed if the full mesh were output.

**BLOCK_SURFACE** This option is similar to the EXPOSED_SURFACE option except that the skinning process is done an element block at a time instead of for the full model. In this option, faces shared between element blocks will appear in the output model.

8.1.1.6 Component Separator Character

```
COMPONENT SEPARATOR CHARACTER = <string>character|NONE
```

The component separator character is used to separate an output-variable base name from any suffixes. For example, the variable stress can have the suffixes xx, yy, etc. By default, the base name is separated from the suffixes with an underscore character so that we have stress_xx, stress_yy, etc. in the results output file.

You can replace the underscore as the default separator by using the above command line. If you wanted to use the period as the separator, then you would use the following command line:
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COMPONENT SEPARATOR CHARACTER = .

For our example with stress, the stress components would then appear in the results output file as stress.xx, stress.yy, etc. If the stress is for a shell element, there is also an integration point suffix preceded, by default, with an underscore. The above command line also resets the underscore character that precedes the integration point suffix. For our example with the stress base name and the underscore replaced by the period, the results file would have stress.xx.01, stress.xx.02, etc., for the shell elements.

You can eliminate the separator with an empty string or NONE.

8.1.1.7 Output Global Variables

GLOBAL VARIABLES = <string>variable_name
  [AS <string>dbase_variable_name
   <string>variable_name AS <string>dbase_variable_name ...]

Any global variable in Presto can be selected for output in the results file by using the GLOBAL VARIABLES command line. The string variable_name is the name of the global variable. The string variable_name can be either a registered variable listed in Section 8.6 or a user-defined variable (see Section 8.1.2 and Section 9.2.4).

With the AS specification, you can specify the variable and select an alias for this variable in the results file. Suppose, for example, you wanted to output the time steps in Presto, which are identified as timestep, with the alias tstep. You would then enter the command line:

GLOBAL VARIABLES = timestep AS tstep

The GLOBAL VARIABLES command line can be used an arbitrary number of times within a RESULTS OUTPUT command block. It is also possible to specify more than one global variable for output on a command line. If you also wanted to output the kinetic energy, which is registered as KineticEnergy, with the alias ke, you would enter the command line:

GLOBAL VARIABLES = timestep as tstep
   KineticEnergy as ke

The specification of an alias is always optional.

8.1.1.8 Set Begin Time for Results Output

START TIME = <real>output_start_time

Using the START TIME command line, you can write output to the results file beginning at time output_start_time. No results will be written before this time. If other commands set times for results (AT TIME, ADDITIONAL TIMES) that are less than output_start_time, those times will be ignored, and results will not be written at those times.
8.1. RESULTS OUTPUT

8.1.1.9 Adjust Interval for Time Steps

TIMESTEP ADJUSTMENT INTERVAL = <integer>steps

This command line is used to specify that the output will be at exactly the times specified. To hit the output times exactly in an explicit, transient dynamics code, it is necessary to adjust the time step as the time approaches an output time. The integer value \textit{steps} in the \texttt{TIMESTEP ADJUSTMENT INTERVAL} command line specifies the number of time steps to look ahead in order to adjust the time step.

If this command line does not appear, results are output at times closest to the specified output times.

8.1.1.10 Output Interval Specified by Time Increment

\texttt{AT TIME <real>time\_begin INCREMENT = <real>time\_increment\_dt}

At the time specified by \texttt{time\_begin}, results will be output every time increment given by the real value \texttt{time\_increment\_dt}.

8.1.1.11 Additional Times for Output

\texttt{ADDITIONAL TIMES = <real>output\_time1 <real>output\_time2 ...}

In addition to any times specified by the command line in Section 8.1.1.10, you can use the \texttt{ADDITIONAL TIMES} command line to specify an arbitrary number of additional output times.

8.1.1.12 Output Interval Specified by Step Increment

\texttt{AT STEP <integer>step\_begin INCREMENT =
 <integer>step\_increment}

At the step specified by \texttt{step\_begin}, results will be output every step increment given by the integer value \texttt{step\_increment}.

8.1.1.13 Additional Steps for Output

\texttt{ADDITIONAL STEPS = <integer>output\_step1
 <integer>output\_step2 ...}

In addition to any steps specified by the command line in Section 8.1.1.12, you can use the \texttt{ADDITIONAL STEPS} command line to specify an arbitrary number of additional output steps.
8.1.14  Set End Time for Results Output

    TERMINATION TIME = <real>termination_time_value

Results will not be written to the results file after time termination_time_value. If other commands set times for results (AT TIME, ADDITIONAL TIMES) that are greater than termination_time_value, those times will be ignored, and results will not be written at those times.

8.1.15  Use Output Scheduler

    USE OUTPUT SCHEDULER <string>scheduler_name

In an analysis with multiple regions, it can be difficult to synchronize output such as results files. To help synchronize output for analyses with multiple regions, you can define an OUTPUT SCHEDULER command block at the domain level. The scheduler can then be referenced in the RESULTS OUTPUT command block via the USE OUTPUT SCHEDULER command line. The string scheduler_name must match a name used in an OUTPUT SCHEDULER command block. See Section 8.5 for a description of using this command block and the USE OUTPUT SCHEDULER command line.

8.1.16  Write Results If System Error Encountered

    OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
                       SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
                       SIGKILL|SIGILL|SIGSEGV

The OUTPUT ON SIGNAL command line is used to initiate the writing of a results file when the system encounters a type of system error. Only one error type in the list of error types should be entered for this command line. Generally, these system errors cause the code to terminate before the code can add any current results output (results output past the last results output time step) to the results output file. If the code encounters the specified type of error during execution, a results file will be written before execution is terminated.

This command line can also be used to force the writing of a results file at some point during execution of the code. Suppose the command line

    OUTPUT ON SIGNAL = SIGUSR2

is included in the input file. While the code is running, a user can execute (from the keyboard) the system command line

    kill -s SIGUSR2 pid

to terminate execution and force the writing of a results file. In the above system command line, pid is the process identifier, which is an integer.

Note that the OUTPUT ON SIGNAL command line is primarily a debugging tool for code developers.
8.1.2 User-Defined Output

BEGIN USER OUTPUT

# mesh-entity set commands
NODE SET = <string_list>nodeset_names
SURFACE = <string_list>surface_names
BLOCK = <string_list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list> surface_names
REMOVE BLOCK = <string list>block_names
#
# compute global result command
COMPUTE GLOBAL <string>results_var_name AS
  <string>SUM|AVERAGE|MAX|MIN OF <string>NODAL|ELEMENT
  <string>value_var_name [(<integer>component_num)]
#
# user subroutine commands
NODE SET SUBROUTINE = <string>subroutine_name |
  SURFACE SUBROUTINE = <string>subroutine_name |
  ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
#
# copy command
COPY ELEMENT VARIABLE <string>ev_name TO NODAL VARIABLE
  <string>nv_name
#
# compute for element death
COMPUTE AT EVERY TIME STEP
#
# additional command
ACTIVE PERIODS = <string list>period_names
END [USER OUTPUT]

The USER OUTPUT command block lets the user generate specialized output information derived from analysis results such as element stresses, displacements, and velocities. For example, the USER OUTPUT command block could be used to sum the contact forces in a particular direction in the global axes and on a certain surface to give a net resultant contact force on that surface. In this example, we essentially postprocess contact information and reduce it to a single value for
a surface (or set of surfaces). This, then, is one of the purposes of the USER OUTPUT command block—to postprocess analysis results as the code is running and produce a reduced set of specialized output information. The USER OUTPUT command block offers an alternative to writing out large quantities of data and then postprocessing them with some external code in order to produce specialized output results. Another use of the USER OUTPUT command block is to generate variables that can be used for element death. An element can be killed by using some criterion based on a user variable defined in the USER OUTPUT command block.

There are three options for calculating user-defined quantities. In the first option, a single command line in the command block is used to compute reductions of registered variables on subsets of the mesh. This option makes use of the COMPUTE GLOBAL command line. The above example of the contact force represents an instance where we can accomplish the desired result simply by using the COMPUTE GLOBAL command line. In the second option, the command block specifies a user subroutine to run immediately preceding output to calculate any desired variable. This option makes use of a NODE SET, SURFACE, or ELEMENT BLOCK SUBROUTINE command line. Finally, there is an option to copy an element variable for an element to the nodes associated with the element, via the COPY ELEMENT VARIABLE command line. This copy option is a specialized option that has been made available primarily for creating results files for some of the postprocessing tools used with Presto. You can use only one of the three options—compute global result, user subroutine, or copy—in a given command block.

For the compute global result option, a user-defined variable is automatically generated. This user-defined variable is given whatever name the user selects for results_var_name in the above specification for the COMPUTE GLOBAL command line. If the user subroutine or copy option is used, the user will need to define some type of user variable with the USER VARIABLE command block described in Section 9.2.4.

User-defined variables, whether they are generated via the compute global result option or the USER VARIABLE command block, are not automatically written to a results or history file. If the user wants to output any user-defined variables, these variables must be referenced in a results or history output specification (see Section 8.1.1 and Section 8.2, which describe the output of variables to results files and history files, respectively). If the user wants to use any user-defined variable for element death, the user must include the COMPUTE AT EVERY TIME STEP command line.

The USER OUTPUT command block contains five groups of commands—mesh-entity set, compute global result, user subroutine, copy, and compute for element death. Each of these command groups is basically independent of the others. In addition to the command lines in the five command groups, there is an additional command line: ACTIVE PERIODS. The following sections provide descriptions of the different command groups and the ACTIVE PERIODS command line.

8.1.2.1 Mesh-Entity Set Commands

The {mesh-entity set commands} portion of the USER OUTPUT command block specifies the nodes, element faces, or elements associated with the variable to be output. This portion of the command block can include some combination of the following command lines:
8.1. RESULTS OUTPUT

NODE SET = <string_list>nodeset_names
SURFACE = <string_list>surface_names
BLOCK = <string_list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list> surface_names
REMOVE BLOCK = <string list>block_names

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes, element faces, or elements. See Section 6.1.1 for more information about the use of these command lines for mesh entities. There must be at least one NODE SET, SURFACE, BLOCK, or INCLUDE ALL BLOCKS command line in the command block.

8.1.2.2 Compute Global Result Command

If the compute global result option is selected, Presto returns a single global value or a set of global values by examining the current values for a named registered nodal or element variable and then calculating the output according to a user-specified operation. A single global value, for example, might be the maximum value of one of the stress components of all the elements in our specified set; a set of global values would be the maximum value of each stress component of all elements in our specified set. Importantly, this option can only be used with a variable that is registered in Presto, not a variable that is created by the user via the USER VARIABLE command block.

The following command line is related to the compute global result option.

```
COMPUTE GLOBAL <string>results_var_name AS
  <string>SUM|AVERAGE|MAX|MIN OF <string>NODAL|ELEMENT
  <string>value_var_name [(<integer>component_num)]
```

In the above command line, the following definitions apply:

- The string results_var_name is the name of a new global variable in which to store the reduced results. To output this variable in a results file, a heartbeat file, or a history file, you will simply use whatever you have selected for results_var_name as the variable name in a GLOBAL VARIABLES command line.

- Four different methods (or reduction types) are available for specifying the operation that will be performed on the values retrieved from the registered variable: SUM, AVERAGE, MAX, and MIN. Only one of these methods can be selected in a GLOBAL COMPUTE command line, however. SUM adds the variable value of all included mesh entities. AVERAGE takes the average value of the variable over all included mesh entities. MAX finds the maximum value over all included mesh entities. MIN finds the minimum value over all included mesh entities.

- The registered variable used to compute the global variable must be either a nodal quantity or an element quantity, as specified by the NODAL or ELEMENT option.
- The string `value_var_name` is the name of the registered variable (see Section 8.6 for a listing of the registered variables).

- There is an optional input, `component_num` (meaning component number), on the command line that allows the user to specify a particular (and single) value that will be returned for the new global variable. If `component_num` is not included in the command line, the global variable will have as many components as the registered variable. For example, if `component_num` was not specified and the registered variable was a displacement (which has three components—`x`, `y`, and `z`), the global variable that is returned would have three values. Each component of the registered variable will be reduced independently and placed in the corresponding position of the returned global variable. In the output file, the returned values will begin with the name of the global variable and be appended with the identification of the kind of component. For example, if `myresults` was specified for `results_var_name` and the registered variable was a displacement, the output values would be displayed as `myresults_x`, `myresults_y`, and `myresults_z`.

Usage of `component_num`, which must be enclosed in parentheses, requires that you enter an integer number that corresponds to the position of the desired value in the set of possible values for the named registered variable. In other words, this number does not indicate how many components are stored for the variable. See the section below titled “Determining the Component Number” for further information on obtaining the required value for `component_num`.

The following is an example of using the `GLOBAL COMPUTE` command line to compute the net `x`-direction reaction force:

```
COMPUTE GLOBAL wall_x_reaction AS SUM OF NODAL reactions(1)
```

**Determining the Component Number:** If you want to specify that a specific value is returned for the global variable, the one named `results_var_name`, select an integer that corresponds to the position of that value in Table 8.4. Thus, for example, if you only wanted the ZZ component of a registered variable that was a symmetric tensor, the value for `component_num` would be specified as “(3)” in the command line.

### 8.1.2.3 User Subroutine Commands

If the user subroutine option is used, the user-defined output quantities will be calculated by a subroutine that is written by the user explicitly for this purpose. The subroutine will be called by Presto at the appropriate time to perform the calculations. User subroutines allow for more generality in computing user-defined results than the `GLOBAL COMPUTE` command line. Suppose, for example, you had an analytic solution for a problem and wanted to compute the difference between some analytic value and a corresponding computed value throughout an analysis. The user subroutine option would allow you to make this comparison. The full details for user subroutines are given in Chapter 9.

The following command lines are related to the user subroutine option:
Table 8.4: Selection of Component Number

<table>
<thead>
<tr>
<th>Variable Type</th>
<th>component_num</th>
<th>Description</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vector</td>
<td>1</td>
<td>X component</td>
<td>A vector has three components. Displacements, for example, are handled as vectors.</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>Y component</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>Z component</td>
<td></td>
</tr>
<tr>
<td>Symmetric Tensor</td>
<td>1</td>
<td>XX component</td>
<td>Symmetric tensors have six components. Stresses for most solid elements are symmetric tensors.</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>YY component</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>ZZ component</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>XY component</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>YZ component</td>
<td></td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>ZX component</td>
<td></td>
</tr>
<tr>
<td>Full Tensor</td>
<td>1</td>
<td>XX component</td>
<td>Full tensors are used occasionally by Presto. Examples include velocity gradients and material rotations.</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>YY component</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>ZZ component</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>XY component</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>YZ component</td>
<td></td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>ZX component</td>
<td></td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>YX component</td>
<td></td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>ZY component</td>
<td></td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>XZ component</td>
<td></td>
</tr>
</tbody>
</table>
The user subroutine option is invoked by using the NODE SET SUBROUTINE command line, the SURFACE SUBROUTINE command line, or the ELEMENT BLOCK SUBROUTINE command line. The particular command line selected depends on the mesh-entity type of the variable for which the result quantities are being calculated. For example, variables associated with nodes would be calculated by using a NODE SET SUBROUTINE command line, variables associated with faces by using a SURFACE SUBROUTINE command line, and variables associated with elements by using the ELEMENT BLOCK SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user. A user subroutine in the USER OUTPUT command block returns no values. Instead, it performs its operations directly with commands such as aupst_put_nodal_var, aupst_put_elem_var, and aupst_put_global_var. Consult with Chapter 9 for further discussion of these various put commands.

Following the selected command line (NODE SET SUBROUTINE, SURFACE SUBROUTINE, or ELEMENT BLOCK SUBROUTINE) are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 9.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided in Chapter 9.

Importantly, to implement the user subroutine option and output the calculated information, you would also need to do the following:

1. Create the user-defined variable with a USER VARIABLE command block.

2. Calculate the results for the user-defined variable in the user subroutine.

3. Write the results for the user-defined variable to an output file by referencing it in a RESULTS OUTPUT command block and/or a HISTORY OUTPUT command block and/or a HEARTBEAT OUTPUT command block. In the RESULTS OUTPUT command block, you would use a NODAL VARIABLES command line, an ELEMENT VARIABLES command line, or a GLOBAL VARIABLES command line, depending on how you defined the variable in the USER VARIABLE command block. Similarly, in the HISTORY OUTPUT or HEARTBEAT OUTPUT command block, you would use the applicable form of the VARIABLE command line, depending on how you defined the variable in the USER VARIABLE command block.
8.1.2.4 Copy Command

COPY ELEMENT VARIABLE <string>ev_name TO NODAL VARIABLE <string>nv_name

The COPY ELEMENT VARIABLE command line copies the value of an element variable to a node associated with the element. The element variable to be copied is specified by ev_name; the name of the nodal variable to which the value is being transferred is nv_name. The nodal variable must be specified as a user-defined variable.

8.1.2.5 Compute at Every Step Command

COMPUTE AT EVERY TIME STEP

If this command line appears in the USER OUTPUT command block, a user-defined variable in the command block will be written at every time step. The COMPUTE AT EVERY TIME STEP command line is required if a user-defined variable is used in a criterion for element death. (Section 9.2.4 discusses user-defined variables, and Section 5.5 discusses element death.) For element death, a user-defined variable must be calculated at every time step.

8.1.2.6 Additional Command

The ACTIVE PERIODS command line can appear as an option in the USER OUTPUT command block:

ACTIVE PERIODS = <string list>period_names

This command line determines when the boundary condition is active. See Section 2.5 for more information about this optional command line.
8.2 History Output

BEGIN HISTORY OUTPUT <string>history_name
  DATABASE NAME = <string>history_file_name
  DATABASE TYPE = <string>database_type(exodusII)
  OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
    (ON|TRUE|YES)
  TITLE <string>user_title
  #
  # for global variables
  VARIABLE = GLOBAL
    <string>variable_name
    [AS <string>history_variable_name]
    #
  # for mesh entity - node, edge, face, element - variables
  VARIABLE =
    NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
    AT NODE|NODAL|EDGE|FACE|ELEMENT <integer>entity_id
    [AS <string>history_variable_name]
    #
  # for nearest point output of mesh entity - node, edge, face, element - variables
  VARIABLE =
    NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
    NEAREST LOCATION <real>global_x,
    <real>global_y>, <real>global_z
    [AS <string>history_variable_name]
  START TIME = <real>output_start_time
  TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
  AT TIME <real>time_begin INCREMENT =
    <real>time_increment_dt
  ADDITIONAL TIMES = <real>output_time1
    <real>output_time2 ...
  AT STEP <integer>step_begin INCREMENT =
    <integer>step_increment
  ADDITIONAL STEPS = <integer>output_step1
    <integer>output_step2 ...
  TERMINATION TIME = <real>termination_time_value
  USE OUTPUT SCHEDULER <string>scheduler_name
  OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
    SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
    SIGILL|SIGILL|SIGSEGV
END [HISTORY OUTPUT <string>history_name]

A history file gives nodal variable results (displacements, forces, etc.) for specific nodes, edge variable results for specific edges, face variable results for specific faces, element results (stress,
8.2. **HISTORY OUTPUT**

strain, etc.) for specific elements, and global results at specified times. You can specify a history file, the results to be included in this file, and the frequency at which results are written by using a **HISTORY OUTPUT** command block. The command block appears inside the region scope. For history output, you will typically work with node and element variables, and, on some occasions, face variables.

More than one history file can be specified for an analysis. For each history file, there will be one **HISTORY OUTPUT** command block. The command block for a history file description begins with:

```
BEGIN HISTORY OUTPUT <string>history_name
```

and is terminated with:

```
END [HISTORY OUTPUT <string>history_name]
```

where **history_name** is a user-selected name for the command block. Nested within the **HISTORY OUTPUT** command block are a set of command lines, as shown in the block summary given above. The first two command lines listed (**DATABASE NAME** and **DATABASE TYPE**) give pertinent information about the history file. The command line

```
DATABASE NAME = <string>history_file_name
```

gives the name of the history file with the string **history_file_name**. If the history file is to appear in the current directory and is named *job.h*, this command line would appear as:

```
DATABASE NAME = job.h
```

If the history file is to be created in some other directory, the command line would have to show the path to that directory.

If the history file does not use the Exodus II format [1], you must specify the format for the history file using the command line:

```
DATABASE TYPE = <string>database_type(exodusII)
```

Currently, both the Exodus II database and the XDMF database [2] are supported in Presto and Adagio. Exodus II is more commonly used than XDMF. Other options may be added in the future.

The **OVERWRITE** command line can be used to prevent the overwriting of existing history files.

```
OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
```

The **OVERWRITE** command line allows only a single value. If you set the value to **FALSE**, **NO**, or **OFF**, the code will terminate before existing history files can be overwritten. If you set the value to **TRUE**, **YES**, or **ON**, then existing history files can be overwritten (the default status). Suppose, for example, that we have an existing history file named *job21.h*. Suppose also that we have an input file with a **HISTORY OUTPUT** command block that contains the **OVERWRITE** command line set to **ON** and the **DATABASE NAME** command line set to:

```
DATABASE NAME = job21.h
```

If you run the code under these conditions, the existing history file *job21.h* will be overwritten.
Whether or not history files are overwritten is also impacted by the use of the automatic read and write option for restart files described in Section 8.4.1.1. If you use the automatic read and write option for restart files, the history files, like the restart files, are automatically managed. The automatic read and write option in restart adds extensions to file names and prevents the overwriting of any existing restart or history files. For the case of a user-controlled read and write of restart files (Section 8.4.1.2) or of no restart, however, the OVERWRITE command line is useful for preventing the overwriting of history files.

You may add a title to the history file by using the TITLE command line. Whatever you specify for the user_title will be written to the history file. Some of the programs that process the history file (such as various SEACAS programs [3]) can read and display this information.

The other command lines that appear in the HISTORY OUTPUT command block determine the type and frequency of information that is output. Descriptions of these command lines follow in Section 8.2.1 through Section 8.2.11. Note that the command lines for controlling the frequency of history output (in Section 8.2.1 through Section 8.2.11) are the same as those for controlling the frequency of results output. These frequency-related command lines are repeated here for convenience.

### 8.2.1 Output Variables

The VARIABLE command line is used to select variables for output in the history file. One of several types of variables—GLOBAL, NODE (or NODAL), EDGE, FACE, or ELEMENT—can be selected for output. The form of the command line varies depending on the type of variable that is selected for output.

#### 8.2.1.1 Global Output Variables

```
VARIABLE = GLOBAL
<string>variable_name
[AS <string>history_variable_name]
```

This form of the VARIABLE command line lets you select any global variable for output in the history file. The variable is selected with the string variable_name. The string variable_name is the name of the global variable and can be either a registered variable listed in Section 8.6 or a user-defined variable (see Section 8.1.2 and Section 9.2.4).

You can also specify an arbitrary name, history_variable_name, for the selected entity following the AS key word. For example, suppose you want to output the kinetic energy (KineticEnergy) as KE. The command line to obtain the kinetic energy in the history file would be

```
VARIABLE = GLOBAL KineticEnergy AS KE
```

The specification of an alias is always optional.
8.2. HISTORY OUTPUT

8.2.1.2 Mesh Entity Output Variables

VARIABLE =
NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
AT NODE|NODAL|EDGE|FACE|ELEMENT <integer>entity_id
[AS <string>history_variable_name]

This form of the VARIABLE command line lets you select any nodal, edge, face, or element variable for a specific mesh entity for output in the history file. For example, this form of the VARIABLE command line will let you pick the displacement at a specific node and output the displacement to the history file using an alias that you have chosen.

For this form of the VARIABLE command line, the mesh entity type following the delimiter (=) is set to NODE (or NODAL), EDGE, FACE, or ELEMENT depending on the variable (set by variable_name) to be output. If the mesh entity type is set to NODE (or NODAL), EDGE, or FACE, the string variable_name can be either a registered variable listed in Section 8.6 or a user-defined variable (see Section 8.1.2 and Section 9.2.4). If the mesh entity type is set to ELEMENT, the string variable_name can be a registered variable listed in Section 8.6, a user-defined variable (see Section 8.1.2 and Section 9.2.4), or a derived output quantity. See the latter portion of Section 8.1.1.4 for a detailed discussion of derived output. A complete list of derived output quantities is given in Tables 8.1, 8.2, and 8.3 in Section 8.1.1.4.

Selection of a specific mesh entity follows the AT key word. You select a mesh entity type (NODE [or NODAL], EDGE, FACE, or ELEMENT) followed by the specific integer identifier, entity_id, for the mesh entity. You can specify an arbitrary name, history_variable_name, for the selected entity following the AS key word. For example, suppose you want to output the accelerations at node 88. The command line to obtain the accelerations at node 88 for the history file would be:

VARIABLE = NODE ACCELERATION AT NODE 88 AS accel_88

where accel_88 is the arbitrary name that will be used for this history variable in the history file.

Note that either the key word NODE or NODAL can be used for nodal quantities. The specification of an alias is always optional.

As an example of derived output, suppose you wanted to output the von Mises stress for solid element 1024. The command line to obtain the von Mises stress for element 1024 for the history file would be:

VARIABLE = ELEMENT VON_MISES AT ELEMENT 1024 AS vm_1024

where vm_1024 is the arbitrary name that will be used for this history variable in the history file.

8.2.1.3 Nearest Point Output Variables

VARIABLE =
NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
NEAREST LOCATION <real>global_x,
  real<global_y>, real<global_z>
[AS <string>history_variable_name]
This form of the VARIABLE command line lets you select any nodal, edge, face, or element variable for output in the history file using a nearest point criterion. The command line described in this subsection is an alternative to the command line described in the preceding section, Section 8.2.1.2, for obtaining history output. The command line in this section or the command line in Section 8.2.1.2 produces history files with variable information. The difference in these two command lines (Section 8.2.1.3 and Section 8.2.1.2) is simply in how the variable information is selected.

For the above form of the VARIABLE command line, the mesh entity type following the delimiter (=) is set to NODE (or NODAL), EDGE, FACE, or ELEMENT depending on the variable (set by variable_name) to be output. If the mesh entity type is set to NODE (or NODAL), EDGE, or FACE, the string variable_name can be either a registered variable listed in Section 8.6 or a user-defined variable (see Section 8.1.2 and Section 9.2.4). If the mesh entity type is set to ELEMENT, the string variable_name can be a registered variable listed in Section 8.6, a user-defined variable (see Section 8.1.2 and Section 9.2.4), or a derived output quantity. See the latter portion of Section 8.1.1.4 for a detailed discussion of derived output. A complete list of derived output quantities is given in Tables 8.1, 8.2, and 8.3 in Section 8.1.1.4.

The specific mesh entity used for output is determined by global coordinates specified by the NEAREST LOCATION key word and its associated input parameters—global_x, global_y, global_z. The specific mesh entity chosen for output is as follows:

- If the mesh entity has been set to NODE (or NODAL), the node in the mesh selected for output is the node whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters global_x, global_y, and global_z.

- If the mesh entity has been set to EDGE, the edge in the mesh selected for output is the edge with a center point (the average location of the two end points of the edge) whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters global_x, global_y, and global_z.

- If the mesh entity has been set to FACE, the face in the mesh selected for output is the face with a centroid whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters global_x, global_y, and global_z.

- If the mesh entity has been set to ELEMENT, the element in the mesh selected for output is the element with a centroid whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters global_x, global_y, and global_z.

Note that, in all the above cases, the original model coordinates are used when selecting the nearest entity, not the current coordinates.

You can specify an arbitrary name, history_variable_name, for the selected entity following the AS key word. As an example, suppose you want to output the accelerations at a node closest to the point with global coordinates (1012.0, 54.86, 103.3141). The command line to obtain the accelerations at the node closest to this location for the history file would be:

VARIABLE = NODE ACCELERATION
NEAREST LOCATION 1012.0, 54.86, 103.3141 AS accel_near
where accel_near is the arbitrary name that will be used for this history variable in the history file.

Note that either the key word NODE or NODAL can be used for nodal quantities. The specification of an alias is always optional.

### 8.2.2 Outputting History Data on a Node Set

It is commonly desired to output history data on a single-node node set. If a mesh file is slightly modified, the node and element numbers will completely change. The node associated with a node set, however, remains the same, i.e., the node in the node set retains the same initial geometric location with the same connectivity to other elements even when its node number changes. Therefore, we might want to specify the history output for a node set with a single node rather than with the global identifier for a node. This can easily be accomplished, as follows:

```plaintext
begin user output
    node set = nodelist_1
    compute global disp_ns_1 as average of nodal displacement
end

begin history output
    variable = global disp_ns_1
end
```

If nodelist_1 contains only a single node, the history output variable disp_ns_1 will contain the displacement for the single node in the node set. If nodelist_1 contains multiple nodes, the average displacement of the nodes will be output.

### 8.2.3 Set Begin Time for History Output

```plaintext
START TIME = <real>output_start_time
```

Using the START TIME command line, you can write history variables to the history file beginning at time output_start_time. No history variables will be written before this time. If other commands set times for history output (AT TIME, ADDITIONAL TIMES) that are less than output_start_time, those times will be ignored, and history output will not be written at those times.

### 8.2.4 Adjust Interval for Time Steps

```plaintext
TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
```
This command line is used to specify that the output will be at exactly the times specified. To hit the output times exactly in an explicit, transient dynamics code, it is necessary to adjust the time step as the time approaches an output time. The integer value steps in the TIMESTEP ADJUSTMENT INTERVAL command line specifies the number of time steps to look ahead in order to adjust the time step.

If this command line does not appear, history variables are output at times closest to the specified output times.

**8.2.5 Output Interval Specified by Time Increment**

\[
\text{AT TIME } \text{time}_\text{begin} \text{ INCREMENT } = \text{time}_\text{increment}_\text{dt}
\]

At the time specified by \text{time}_\text{begin}, history variables will be output every time increment given by the real value \text{time}_\text{increment}_\text{dt}.

**8.2.6 Additional Times for Output**

\[
\text{ADDITIONAL TIMES } = \text{output}_\text{time1} \text{output}_\text{time2} \ldots
\]

In addition to any times specified by the command line in Section 8.2.5, you can use the ADDITIONAL TIMES command line to specify an arbitrary number of additional output times.

**8.2.7 Output Interval Specified by Step Increment**

\[
\text{AT STEP } \text{step}_\text{begin} \text{ INCREMENT } = \text{step}_\text{increment}
\]

At the step specified by \text{step}_\text{begin}, history variables will be output every step increment given by the integer value \text{step}_\text{increment}.

**8.2.8 Additional Steps for Output**

\[
\text{ADDITIONAL STEPS } = \text{output}_\text{step1} \text{output}_\text{step2} \ldots
\]

In addition to any steps specified by the command line in Section 8.2.7, you can use the ADDITIONAL STEPS command line to specify an arbitrary number of steps.
8.2.9  Set End Time for History Output

\[ \text{TERMINATION TIME} = \text{termination\_time\_value} \]

History output will not be written to the history file after time \( \text{termination\_time\_value} \). If other commands set times for history output (AT TIME, ADDITIONAL TIMES) that are greater than \( \text{termination\_time\_value} \), those times will be ignored, and history output will not be written at those times.

8.2.10  Use Output Scheduler

\[ \text{USE OUTPUT SCHEDULER} \ <\text{string}>\text{scheduler\_name} \]

In an analysis with multiple regions, it can be difficult to synchronize output such as history files. To help synchronize output for analyses with multiple regions, you can define an OUTPUT SCHEDULER command block at the domain level. The scheduler can then be referenced in the HISTORY OUTPUT command block via the USE OUTPUT SCHEDULER command line. The string \( \text{scheduler\_name} \) must match a name used in an OUTPUT SCHEDULER command block. See Section 8.5 for a description of using this command block and the USE OUTPUT SCHEDULER command line.

8.2.11  Write History If System Error Encountered

\[ \text{OUTPUT ON SIGNAL} = \ <\text{string}>\text{SIGALRM}|\text{SIGFPE}|\text{SIGHUP}|\text{SIGINT}|\]
\[ \text{SIGPIPE}|\text{SIGQUIT}|\text{SIGTERM}|\text{SIGUSR1}|\text{SIGUSR2}|\text{SIGABRT}|\]
\[ \text{SIGKILL}|\text{SIGILL}|\text{SIGSEGV} \]

The OUTPUT ON SIGNAL command line is used to initiate the writing of a history file when the system encounters a type of system error. Only one error type in the list of error types should be entered for this command line. Generally, these system errors cause the code to terminate before the code can add any current history output (history output past the last history output time step) to the history file. If the code encounters the specified type of error during execution, a history file will be written before execution is terminated.

This command line can also be used to force the writing of a history file at some point during execution of the code. Suppose the command line

\[ \text{OUTPUT ON SIGNAL} = \text{SIGUSR2} \]

is included in the input file. While the code is running, a user can execute (from the keyboard) the system command line

\[ \text{kill} -s \text{SIGUSR2} \ <\text{pid}> \]

\( \text{pid} \) is the process identifier, which is an integer.
Note that the `OUTPUT ON SIGNAL` command line is primarily a debugging tool for code developers.
BEGIN HEARTBEAT OUTPUT <string>heartbeat_name
    # Can also use predefined streams "cout", "stdout",
    # "cerr", "clog", "log", "output", or "outputP0"
    STREAM NAME = <string>heartbeat_file_name
    
    # for global variables
    VARIABLE = GLOBAL
    <string>variable_name
    [AS <string>heartbeat_variable_name]
    
    # for mesh entity - node, edge, face,
    # element - variables
    VARIABLE =
        NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
        AT NODE|NODAL|EDGE|FACE|ELEMENT <integer>entity_id
        [AS <string>heartbeat_variable_name]
    
    # for nearest point output of mesh entity - node,
    # edge, face, element - variables
    VARIABLE =
        NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
        NEAREST LOCATION <real>global_x,
        <real>global_y>, <real>global_z
        [AS <string>heartbeat_variable_name]
    START TIME = <real>output_start_time
    TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
    AT TIME <real>time_begin INCREMENT =
        <real>time_increment_dt
    ADDITIONAL TIMES = <real>output_time1
    <real>output_time2 ...
    AT STEP <integer>step_begin INCREMENT =
        <integer>step_increment
    ADDITIONAL STEPS = <integer>output_step1
    <integer>output_step2 ...
    TERMINATION TIME = <real>termination_time_value
    USE OUTPUT SCHEDULER <string>scheduler_name
    OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
                       SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
                       SIGKILL|SIGILL|SIGSEGV
    PRECISION = <integer>precision
    LABELS = <string>OFF|ON
    LEGEND = <string>OFF|ON
    TIMESTAMP FORMAT <string>timestamp_format
    MONITOR = <string>RESULTS|RESTART|HISTORY
END [HEARTBEAT OUTPUT <string>heartbeat_name]
The heartbeat output is text output that gives:

- nodal variable results (displacements, forces, etc.) for specific nodes,
- edge variable results for specific edges,
- face variable results for specific faces,
- element results (stress, strain, etc.) for specific elements, and
- global results

at specified times.

**Known Issue:** User defined variables (see Section 9.2.4) are not currently supported with heartbeat output.

The output is written as text instead of the binary history output. You can specify a heartbeat file, the results to be included in this file, the formatting of the output, and the frequency at which results are written by using a `HEARTBEAT OUTPUT` command block. The command block appears inside the region scope. For heartbeat output, you will typically work with global, node, and element variables, and, on some occasions, face variables.

More than one heartbeat file can be specified for an analysis. For each heartbeat file, there will be one `HEARTBEAT OUTPUT` command block. The command block for a heartbeat file description begins with

```
BEGIN HEARTBEAT OUTPUT <string>heartbeat_name
```

and is terminated with

```
END [HEARTBEAT OUTPUT <string>heartbeat_name]
```

where `heartbeat_name` is a user-selected name for the command block. Nested within the `HEARTBEAT OUTPUT` command block are a set of command lines, as shown in the block summary given above. The first command line listed (STREAM NAME) gives pertinent information about the heartbeat file. The command line

```
STREAM NAME = <string>heartbeat_file_name
```

gives the name of the heartbeat file with the string `heartbeat_file_name`. If the file already exists, it is overwritten. If the heartbeat file is to appear in the current directory and is named `job.h`, this command line would appear as

```
STREAM NAME = job.h
```

If the heartbeat file is to be created in some other directory, the command line would have to show the absolute path to that directory.

In addition to specifying a specific filename, there are several predefined streams that can be specified. The predefined streams are:
8.3. HEARTBEAT OUTPUT

- `cout` or `stdout` specifies standard output;
- `cerr`, `stderr`, `clog`, or `log` specifies standard error;
- `output` or `output0` specifies Sierra’s standard output which is redirected to the file specified by the `-o` option on the command line.

The other command lines that appear in the HEARTBEAT OUTPUT command block determine the type, frequency, and format of information that is output. Descriptions of these command lines follow in Section 8.3.1 through Section 8.3.13. Note that the command lines for controlling the frequency of heartbeat output (in Section 8.3.3 through Section 8.3.11) are the same as those for controlling the frequency of results and history output. These frequency-related command lines are repeated here for convenience.

### 8.3.1 Output Variables

The VARIABLE command line is used to select variables for output in the heartbeat file. One of several types of variables—GLOBAL, NODE (or NODAL), EDGE, FACE, or ELEMENT—can be selected for output. The form of the command line varies depending on the type of variable that is selected for output.

#### 8.3.1.1 Global Output Variables

```
VARIABLE = GLOBAL
<string>variable_name
[AS <string>heartbeat_variable_name]
```

This form of the VARIABLE command line lets you select any global variable for output in the heartbeat file. The variable is selected with the string variable_name. The string variable_name is the name of the global variable and can be either a registered variable listed in Section 8.6 or a user-defined variable (see Section 8.1.2 and Section 9.2.4). The variable_name can also specify time, timestep, or step to output the current simulation time, timestep, or execution step, respectively.

You can also specify an arbitrary name, heartbeat_variable_name, for the selected entity following the AS key word. For example, suppose you want to output the kinetic energy (KineticEnergy) as KE. The command line to obtain the kinetic energy in the heartbeat file would be:

```
VARIABLE = GLOBAL KineticEnergy AS KE
```

The specification of an alias is always optional.

#### 8.3.1.2 Mesh Entity Output Variables

```
VARIABLE =
```
This form of the \texttt{VARIABLE} command line lets you select any nodal, edge, face, or element variable for a specific mesh entity for output in the heartbeat file. For example, this form of the \texttt{VARIABLE} command line will let you pick the displacement at a specific node and output the displacement to the heartbeat file using an alias that you have chosen.

For this form of the \texttt{VARIABLE} command line, the mesh entity type following the delimiter (\texttt{=} ) is set to \texttt{NODE} (or \texttt{NODAL}), \texttt{EDGE}, \texttt{FACE}, or \texttt{ELEMENT} depending on the variable (set by \texttt{variable_name}) to be output. If the mesh entity type is set to \texttt{NODE} (or \texttt{NODAL}), \texttt{EDGE}, or \texttt{FACE}, the string \texttt{variable_name} can be either a registered variable listed in Section 8.6 or a user-defined variable (see Section 8.1.2 and Section 9.2.4). If the mesh entity type is set to \texttt{ELEMENT}, the string \texttt{variable_name} can be a registered variable listed in Section 8.6, a user-defined variable (see Section 8.1.2 and Section 9.2.4), or a derived output quantity. See the latter portion of Section 8.1.1.4 for a detailed discussion of derived output. A complete list of derived output quantities is given in Tables 8.1, 8.2, and 8.3 in Section 8.1.1.4.

Selection of a specific mesh entity follows the \texttt{AT} key word. You select a mesh entity type (\texttt{NODE} [or \texttt{NODAL}], \texttt{EDGE}, \texttt{FACE}, or \texttt{ELEMENT}) followed by the specific integer Identifier, \texttt{entity_id}, for the mesh entity. You can specify an arbitrary name, \texttt{heartbeat_variable_name}, for the selected entity following the \texttt{AS} key word. For example, suppose you want to output the accelerations at node 88. The command line to obtain the accelerations at node 88 for the heartbeat file would be:

\begin{verbatim}
VARIABLE = NODE ACCELERATION AT NODE 88 AS accel_88
\end{verbatim}

where \texttt{accel_88} is the arbitrary name that will be used for this heartbeat variable in the heartbeat file.

Note that either the key word \texttt{NODE} or \texttt{NODAL} can be used for nodal quantities. The specification of an alias is always optional.

As an example of derived output, suppose you wanted to output the von Mises stress for solid element 1024. The command line to obtain the von Mises stress for element 1024 for the heartbeat file would be:

\begin{verbatim}
VARIABLE = ELEMENT VON_MISES AT ELEMENT 1024 AS vm_1024
\end{verbatim}

where \texttt{vm_1024} is the arbitrary name that will be used for this heartbeat variable in the heartbeat file.

\subsection{Nearest Point Output Variables}

\begin{verbatim}
VARIABLE = 
NODE\|NODAL\|EDGE\|FACE\|ELEMENT <string>variable_name 
NEAREST LOCATION <real>global_x, 
    real<global_y>, real<global_z> 
[AS <string>heartbeat_variable_name]
\end{verbatim}
This form of the VARIABLE command line lets you select any nodal, edge, face, or element variable for output in the heartbeat file using a nearest point criterion. The command line described in this subsection is an alternative to the command line described in the preceding section, Section 8.3.1.2, for obtaining heartbeat output. The command line in this section or the command line in Section 8.3.1.2 produces heartbeat files with variable information. The difference in these two command lines (Section 8.3.1.3 and Section 8.3.1.2) is simply in how the variable information is selected.

For the above form of the VARIABLE command line, the mesh entity type following the delimiter (=) is set to NODE (or NODAL), EDGE, FACE, or ELEMENT depending on the variable (set by variable_name) to be output. If the mesh entity type is set to NODE (or NODAL), EDGE, or FACE, the string variable_name can be either a registered variable listed in Section 8.6 or a user-defined variable (see Section 8.1.2 and Section 9.2.4). If the mesh entity type is set to ELEMENT, the string variable_name can be a registered variable listed in Section 8.6, a user-defined variable (see Section 8.1.2 and Section 9.2.4), or a derived output quantity. See the latter portion of Section 8.1.1.4 for a detailed discussion of derived output. A complete list of derived output quantities is given in Tables 8.1, 8.2, and 8.3 in Section 8.1.1.4.

The specific mesh entity used for output is determined by global coordinates specified by the NEAREST LOCATION key word and its associated input parameters—global_x, global_y, global_z. The specific mesh entity chosen for output is as follows:

- If the mesh entity has been set to NODE (or NODAL), the node in the mesh selected for output is the node whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters global_x, global_y, and global_z.

- If the mesh entity has been set to EDGE, the edge in the mesh selected for output is the edge with a center point (the average location of the two end points of the edge) whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters global_x, global_y, and global_z.

- If the mesh entity has been set to FACE, the face in the mesh selected for output is the face with a centroid whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters global_x, global_y, and global_z.

- If the mesh entity has been set to ELEMENT, the element in the mesh selected for output is the element with a centroid whose initial position is nearest the input global X, Y, and Z coordinates specified with the parameters global_x, global_y, and global_z.

Note that, in all the above cases, the original model coordinates are used when selecting the nearest entity, not the current coordinates.

You can specify an arbitrary name, heartbeat_variable_name, for the selected entity following the AS key word. As an example, suppose you want to output the accelerations at a node closest to the point with global coordinates (1012.0, 54.86, 103.3141). The command line to obtain the accelerations at the node closest to this location for the heartbeat file would be:

```
VARIABLE = NODE ACCELERATION
NEAREST LOCATION 1012.0, 54.86, 103.3141 AS accel_near
```
where `accel_near` is the arbitrary name that will be used for this heartbeat variable in the heartbeat file.

Note that either the key word `NODE` or `NODAL` can be used for nodal quantities. The specification of an alias is always optional.

### 8.3.2 Outputting Heartbeat Data on a Node Set

It is commonly desired to output heartbeat data on a single-node node set. If a mesh file is slightly modified, the node and element numbers will completely change. The node associated with a node set, however, remains the same, i.e., the node in the node set retains the same initial geometric location with the same connectivity to other elements even when its node number changes. Therefore, we might want to specify the heartbeat output for a node set with a single node rather than with the global identifier for a node. This can easily be accomplished, as follows:

```plaintext
begin user output
  node set = nodelist_1
  compute global disp_ns_1 as average of nodal displacement
end

begin heartbeat output
  variable = global disp_ns_1
end
```

If `nodelist_1` contains only a single node, the heartbeat output variable `disp_ns_1` will contain the displacement for the single node in the node set. If `nodelist_1` contains multiple nodes, the average displacement of the nodes will be output.

### 8.3.3 Set Begin Time for Heartbeat Output

```
START TIME = <real>output_start_time
```

Using the `START TIME` command line, you can write heartbeat variables to the heartbeat file beginning at time `output_start_time`. No heartbeat variables will be written before this time. If other commands set times for heartbeat output (`AT TIME`, `ADDITIONAL TIMES`) that are less than `output_start_time`, those times will be ignored, and heartbeat output will not be written at those times.

### 8.3.4 Adjust Interval for Time Steps

```
TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
```
This command line is used to specify that the output will be at exactly the times specified. To hit the output times exactly in an explicit, transient dynamics code, it is necessary to adjust the time step as the time approaches an output time. The integer value steps in the TIMESTEP ADJUSTMENT INTERVAL command line specifies the number of time steps to look ahead in order to adjust the time step.

If this command line does not appear, heartbeat variables are output at times closest to the specified output times.

### 8.3.5 Output Interval Specified by Time Increment

\[ \text{AT TIME } \text{time\_begin INCREMENT } = \text{time\_increment\_dt} \]

At the time specified by time\_begin, heartbeat variables will be output every time increment given by the real value time\_increment\_dt.

### 8.3.6 Additional Times for Output

\[
\text{ADDITIONAL TIMES } = \text{output\_time1 output\_time2 \ldots}
\]

In addition to any times specified by the command line in Section 8.3.5, you can use the ADDITIONAL TIMES command line to specify an arbitrary number of additional output times.

### 8.3.7 Output Interval Specified by Step Increment

\[ \text{AT STEP } \text{step\_begin INCREMENT } = \text{step\_increment} \]

At the step specified by step\_begin, heartbeat variables will be output every step increment given by the integer value step\_increment.

### 8.3.8 Additional Steps for Output

\[
\text{ADDITIONAL STEPS } = \text{output\_step1 output\_step2 \ldots}
\]

In addition to any steps specified by the command line in Section 8.2.7, you can use the ADDITIONAL STEPS command line to specify an arbitrary number of steps.
8.3.9 Set End Time for Heartbeat Output

TERMINATION TIME = <real>termination_time_value

Heartbeat output will not be written to the heartbeat file after time termination_time_value. If other commands set times for heartbeat output (AT TIME, ADDITIONAL TIMES) that are greater than termination_time_value, those times will be ignored, and heartbeat output will not be written at those times.

8.3.10 Use Output Scheduler

USE OUTPUT SCHEDULER <string>scheduler_name

In an analysis with multiple regions, it can be difficult to synchronize output such as heartbeat files. To help synchronize output for analyses with multiple regions, you can define an OUTPUT SCHEDULER command block at the domain level. The scheduler can then be referenced in the HEARTBEAT OUTPUT command block via the USE OUTPUT SCHEDULER command line. The string scheduler_name must match a name used in an OUTPUT SCHEDULER command block. See Section 8.5 for a description of using this command block and the USE OUTPUT SCHEDULER command line.

8.3.11 Write Heartbeat On Signal

OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|SIGKILL|SIGILL|SIGSEGV

The OUTPUT ON SIGNAL command line is used to initiate the writing of a heartbeat file when the system encounters the specified signal. The signal can either occur as the result of a system error, or the user can explicitly send the specified signal to the application (See the system documentation man pages for “signal” or “kill” for more information). Only one signal type in the list of signal types should be entered for this command line. Generally, these signals cause the code to terminate before the code can add any current heartbeat output (heartbeat output past the last heartbeat output time step) to the heartbeat file. If the code encounters the specified type of error during execution, a heartbeat file will be written before execution is terminated.

This command line can also be used to force the writing of a heartbeat file at some point during execution of the code. Suppose the command line

OUTPUT ON SIGNAL = SIGUSR2

is included in the input file. While the code is running, a user can execute (from the keyboard) the system command line

kill -s SIGUSR2 pid
to force the writing of a results file. In the above system command line, \( pid \) is the process identifier, which is an integer.

Note that the \texttt{OUTPUT ON SIGNAL} command line is primarily a debugging tool for code developers.

### 8.3.12 Heartbeat Output Formatting Commands

There are several command lines for the heartbeat section that modify the formatting of the heartbeat text output. The default output for the heartbeat data consists of a line beginning with a timestamp showing the current wall-clock time followed by multiple columns of data, for example:

```
Begin HeartBeat Region_1_Heartbeat
Stream Name = output
At Step 0, Increment = 10

precision is 5

Variable = global step
Variable = global timestep as dt
Variable = global time
Variable = global total_energy as te
End
```

```
```

The above example begins each line with a timestamp followed by five labelled data columns. The precision of the real data is 5. There is no legend in the above example. This format can be modified with the following commands.

#### 8.3.12.1 Specify floating point precision

```
PRECISION = <integer>precision
```

By default, the real data is written with a precision of 5 which gives 5 digits following the decimal point. This can be altered with the \texttt{PRECISION} command. If the command line \texttt{PRECISION = 2} is specified, then the above data would look like:

```
Begin HeartBeat Region_1_Heartbeat
```
... precision = 2 ...

End


Note that the precision applies to all real data; it is not possible to specify a different precision for each variable.

8.3.12.2 Specify Labelling of Heartbeat Data

LABELS = <string>OFF|ON

The above example shows the default output which consists of a label and the data separated by “=". The existence of the labels is controlled with the LABELS command. If LABELS = OFF is specified, then the above data would look like:

Begin HeartBeat Region_1_Heartbeat
...
labels = off
precision = 2
...
End

+ [12:17:37] 240, 3.14e-04, 7.57e-02, 4.03e-06
+ [12:17:37] 250, 3.14e-04, 7.88e-02, 1.32e-06

8.3.12.3 Specify Existance of Legend for Heartbeat Data

LEGEND = <string>OFF|ON

Outputting the data without labels can make it easier to work with the data in a spreadsheet program or other data manipulation program, but with no labels, it is difficult to determine what the data really represents. The LEGEND output will print a line at the beginning of the heartbeat output identifying the data in each column. For example:

Begin HeartBeat Region_1_Heartbeat
...
legend = on
labels = off
    precision = 2
...
End
8.3. HEARTBEAT OUTPUT

8.3.12.4 Specify format of timestamp

    TIMESTAMP FORMAT <string>"timestamp_format"

Each line of the heartbeat output is preceded by a timestamp which shows the wall-clock time at the time that the line was output. This can be useful to verify that the code is still running and producing output and to determine how fast the code is running. The default timestamp is in the format “[12:34:56]” which is specified by the format [%H:%M:%S]. If a different format is desired, it can be specified with the TIMESTAMP FORMAT command line. The format must be surrounded by double or single quotes and the format is defined to be the string between the first single or double quote and the last matching quote type. If you want to modify the format, see the documentation for the UNIX strftime command for details on how to specify the format. The example below shows a timestamp format delimited by “{” and “}”. The timestamp consists of an ISO-8601 date format followed by the current time.

    ... timestamp format "{%F %H:%M:%S}" ...
    +{2008-03-17 09:26:17} 2212, 1.34244e-06, 2.96948e-03, 2.96948e-03
    +{2008-03-17 09:26:17} 2213, 1.34244e-06, 2.97082e-03, 2.97082e-03
    +{2008-03-17 09:26:17} 2214, 1.34244e-06, 2.97216e-03, 2.97216e-03
    +{2008-03-17 09:26:17} 2215, 1.34244e-06, 2.97350e-03, 2.97350e-03
    +{2008-03-17 09:26:17} 2216, 1.34244e-06, 2.97485e-03, 2.97485e-03

8.3.13 Monitor Output Events

    MONITOR = <string>RESULTS|RESTART|HISTORY

It is sometimes a benefit to know when the code has written a new set of data to one of the other output files (restart output, history output, or results output). The heartbeat output will report this data if the MONITOR command line is specified. Each time output is performed to any of the monitored output types, a line will be written to the heartbeat file specifying the timestamp, the simulation time and step, and the label name of the output type. For example:

    begin results output my_results
      at step 0, increment = 10
    ...
    end results output results
begin heartbeat data hb
  stream name = stdout
  monitor = results
  labels = off
  legend = on
  timestamp format "%F %H:%M:%S "
at step 0, increment = 2
  variable = global step
  variable = global timestep as dt
  variable = global time
  variable = element spring_engineering_strain at \#
    element 1 as sp1
end

Will give the following output:

....
-2008-03-17 10:03:22 Results data written at time = 0.00096656, step = 720. my_results
+2008-03-17 10:03:22  726, 1.34244e-06, 9.74611e-04, 9.74611e-04
-2008-03-17 10:03:22 Results data written at time = 0.00097998, step = 730. my_results
....
8.4 Restart Data

BEGIN RESTART DATA <string>restart_name
DATABASE NAME = <string>restart_file
INPUT DATABASE NAME = <string>restart_input_file
OUTPUT DATABASE NAME = <string>restart_output_file
DATABASE TYPE = <string>database_type(exodusII)
OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
(ON|TRUE|YES)
START TIME = <real>restart_start_time
TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
AT TIME <real>time_begin INCREMENT =
<real>time_increment_dt
ADDITIONAL TIMES = <real>output_time1
<real>output_time2 ...
AT STEP <integer>step_begin INCREMENT =
<integer>step_increment
ADDITIONAL STEPS = <integer>output_step1
<integer>output_step2 ...
TERMINATION TIME = <real>termination_time_value
OVERLAY COUNT = <integer>overlay_count
CYCLE COUNT = <integer>cycle_count
USE OUTPUT SCHEDULER <string>scheduler_name
OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
SIGILL|SIGSEG
END [RESTART DATA <string>restart_name]

You can specify restart files, either to be written to or read from, and the frequency at which restarts
are written by using a RESTART DATA command block. The command block appears inside the
region scope. To initiate a restart, the RESTART TIME command line (see Section 2.1.3.1) or the
RESTART command line (see Section 2.1.3.2) must also be used. These command lines appear in
the domain scope.

NOTE: In addition to the times at which you request restart information to be written, restart
information is automatically written when an element inverts.

The RESTART DATA command block begins with the input line:

BEGIN RESTART DATA <string>restart_name

and is terminated with:

END [RESTART DATA <string>restart_name]

where restart_name is a user-selected name for the RESTART DATA command block.

Nested within the RESTART DATA command block are a set of command lines, as shown in the
block summary given above.

We begin the discussion of the RESTART DATA command block with various options regarding the
use of restart in general. In Section 8.4.1, you will learn how to use the DATABASE NAME, INPUT DATABASE NAME, OUTPUT DATABASE NAME, and DATABASE TYPE command lines. Usage of the first three of these command lines is tied to the two restart-related command lines RESTART and RESTART TIME, which are found in the domain scope.

Section 8.4.2 discusses use of the OVERWRITE command line, which will prevent or allow the overwriting of existing restart files. (Note that this command line also appears in the command blocks for results output and history output.)

The other command lines that appear in the RESTART DATA command block determine the frequency at which restarts are written. Descriptions of these command lines follow in Section 8.4.3 through Section 8.4.13. Note that the command lines for controlling the frequency of restart output are the same as those for controlling the frequency of results output and history output. These frequency-related command lines are repeated here for convenience.

### 8.4.1 Restart Options

```plaintext
DATABASE NAME = <string>restart_file
INPUT DATABASE NAME = <string>restart_input_file
OUTPUT DATABASE NAME = <string>restart_output_file
DATABASE TYPE = <string>database_type(exodusII)
```

You can read from and create restart files in an automated fashion, the preferred method, or you can carefully control how you read from and create restart files. In our discussion of the overall options for the use of restart, we begin with the first three command lines listed above (DATABASE NAME, INPUT DATABASE NAME, and OUTPUT DATABASE NAME). All three of these command lines specify a parameter that is a file name or a directory path and file name. If the parameter begins with the “/” character, it is an absolute path; otherwise, the path to the current directory will be prepended to the parameter on the command line. Suppose, for example, that we want to work with a restart file named `component.rst` in the current directory. If we are using the DATABASE NAME command line, then this command line would appear as:

```plaintext
DATABASE NAME = component.rst
```

If we wanted to read or create files in some other directory, the command line would have to show the path to that directory in addition to our file name.

The DATABASE NAME command line will let you read restart information and write restart information to the same file. Section 8.4.1.1 through Section 8.4.1.4 show how this command line is used in particular instances.

You can specify a restart file to read from by using the command line:

```plaintext
INPUT DATABASE NAME = <string>restart_input_file
```

You can specify a restart file to write to by using the command line:

```plaintext
OUTPUT DATABASE NAME = <string>restart_output_file
```

Note that you must use either a DATABASE NAME command line or the INPUT DATABASE NAME
command line/OUTPUT DATABASE NAME command line pair, but not both, in a RESTART DATA command block.

If the restart file does not use the Exodus II format [1], you must specify the format for the results file using the DATABASE TYPE command line:

```
DATABASE TYPE = <string>database_type(exodusII)
```

Currently, the Exodus II database and the XDMF database [2] are supported in Presto and Adagio. Exodus II is more commonly used than XDMF. Other options may be added in the future.

### 8.4.1.1 Automatic Read and Write of Restart Files

You can use the restart option in an automated fashion by using a combination of the RESTART command line in the domain scope and the DATABASE NAME command line in the RESTART DATA command block. This automated use of restart can best be explained by an example. We will use a two-processor example and assume all files will be in our current directory.

The option of automated restart will not only manage the restart files to prevent overwriting, it will also manage the results files and history files to prevent overwriting. In the example we give, we will assume our run includes a RESULTS OUTPUT command block with the command line

```
DATABASE NAME = rslt.e
```

to generate results files with the root file name rslt.e. We will also assume a run includes a HISTORY OUTPUT command block with the command line

```
DATABASE NAME = hist.h
```

to generate history files with the root file name hist.h.

For the first run in our restart sequence, we will have the command line

```
RESTART = AUTOMATIC
```

in the domain scope of our input file. In a TIME STEPPING command block, which is embedded in a TIME CONTROL command block (Section 3.1.1) in the procedure scope of our input file, we will have the command line:

```
START TIME = 0.0
```

In the TIME CONTROL command block we will have the command line

```
TERMINATION TIME = 2.5E-3
```

to set the limits for the begin and end times of the first restart run. These time-related command lines should not be confused with the START TIME and TERMINATION TIME command lines that appear in the RESTART DATA command block.

Finally, for the first run in our restart sequence, the RESTART DATA command block in our input file will be as follows:

```
BEGIN RESTART DATA PRESTO_RESTART
   DATABASE NAME = g.rsout
```
In this block, the DATABASE NAME command line specifies a root file name for the restart file. The AT TIME command line gives the time when we will start to write the restart information and the interval at which the restart information will be written (see Section 8.4.5).

For our first run, the automatic restart option will generate the following restart files:

```
# restart files
g.rsout.2.0
g.rsout.2.1
# results files
rslt.e.2.0
rslt.e.2.1
# history files
hist.h.2.0
hist.h.2.1
```

For the above files, there are extensions on the file names that indicate we have a two-processor run. The 2.0 and 2.1 extensions associate the restart files with the corresponding individual mesh files on each processor. (If our mesh file is mesh.g, then our mesh files on the individual processors will be mesh.g.2.0 and mesh.g.2.1.) All restart information in the above files appears at time intervals of $0.25 \times 10^{-3}$, and the last restart information is written at time $2.5 \times 10^{-3}$. We have also listed the results and history files that will be generated for this run due to the file definitions in the command blocks for the results and history files.

For the second run in our sequence of restart runs, we want to start at the previous termination time, $2.5 \times 10^{-3}$, and terminate at time $5.0 \times 10^{-3}$. We leave everything in our input file (including the START TIME = 0.0 command line in the TIME STEPPING command block, the RESTART command line, and the RESTART DATA command block) the same except for the TERMINATION TIME command line (in the TIME CONTROL command block). The TERMINATION TIME command line will now become:

```
TERMINATION TIME = 5.0E-3
```

It is important to note here that the actual start time for the second run in our analysis is now set by the last time ($2.5 \times 10^{-3}$) that restart information was written. The command line START TIME = 0.0 in the TIME STEPPING command block is now superseded as the actual starting time for the second run by the restart commands. Any START TIME command line in a TIME STEPPING command block is still valid in terms of defining time stepping blocks (these blocks being used to set activation periods), but the restart process sets the actual start time for our analysis. This pattern of control for setting the actual start time holds for any run in our sequence of restart runs.

For the second run in our sequence of restart runs, the restart files will be from time $2.5 \times 10^{-3}$ to time $5.0 \times 10^{-3}$. The restart files in our current directory after the second run will be as follows:

```
# restart files
```
8.4. RESTART DATA

Notice that we have generated new restart files with a `-s0002` extension in addition to the extension associated with the individual processors. All restart information in the above files with the `-s0002` extension appears at time intervals of $0.25 \times 10^{-3}$, the restart information is written between time $2.5 \times 10^{-3}$ and time $5.0 \times 10^{-3}$, and the final restart information is written at time $5.0 \times 10^{-3}$. The restart files for the first run in our sequence of restart runs, `g.rsout.2.0` and `g.rsout.2.1`, have been preserved. New results and history files have been created using the same extension, `-s0002`, as that used for the restart files. The original results and history files have been preserved.

Now, we want to do a third run in our sequence of restart runs. For the third run in our sequence of restart runs, we want to start at the previous termination time, $5.0 \times 10^{-3}$, and terminate at time $8.5 \times 10^{-3}$. We leave everything in our input file (including the START TIME command line, the RESTART command line, and the RESTART DATA command block) the same except for the TERMINATION TIME command line. The TERMINATION TIME command line (within the TIME CONTROL command block) will now become:

\[ \text{TERMINATION TIME} = 8.5 \times 10^{-3} \]

For the third run in our sequence of restart runs, the restart files will be from time $5.0 \times 10^{-3}$ to time $8.5 \times 10^{-3}$. The restart files in our current directory after the third run will be as follows:

```
# restart files
g.rsout.2.0
  g.rsout.2.1
  g.rsout-s0002.2.0
  g.rsout-s0002.2.1
# results files
rslt.e.2.0
  rslt.e.2.1
  rslt.e-s0002.2.0
  rslt.e-s0002.2.1
```

# history files
hist.h.2.0
  hist.h.2.1
  hist.h-s0002.2.0
  hist.h-s0002.2.1
Notice that we have generated new restart files with a -s0003 extension in addition to the extension associated with the individual processors. All restart information in the above files with the -s0003 extension appears at time intervals of 0.25 x 10^{-3}, the restart information is written between time 5.0 x 10^{-3} and time 8.5 x 10^{-3}, and the final restart information is written at time 8.5 x 10^{-3}. The restart files for the first and second runs in our sequence of restart runs have been preserved. New results and history files have been created using the same extension, -s0003, as that used for the restart files. The original results and history files have been preserved.

The process just described can be continued as long as necessary. We will continue the process of generating new restart files with extensions that indicate their place in the sequence of runs.

### 8.4.1.2 User-Controlled Read and Write of Restart Files

You can use the restart option and select specific restart times and specific restart files to read from and write to by using a combination of the **RESTART TIME** command line in the domain scope and the **INPUT DATABASE NAME** and **OUTPUT DATABASE NAME** command line in the **RESTART DATA** command block. This “controlled” use of restart can best be explained by an example. We will use a two-processor example and assume all files will be in our current directory. In this example, we will manage the creation of new restart files so as not to overwrite existing restart files. Unlike the automated option for restart, this controlled use of restart requires that the user manage restart file names so as to prevent overwriting previously generated restart files. The same is true for the results and history files. The user will have to manage the creation of new results and history files so as not to overwrite existing results and history files. Creating new results and history files for each run in the sequence of restart runs requires changing the **DATABASE NAME** command line in the **RESULTS OUTPUT** and **HISTORY OUTPUT** command blocks. We will not show examples for use of the **DATABASE NAME** command line in the **RESULTS OUTPUT** and **HISTORY OUTPUT** command blocks here, as the actual use of the **DATABASE NAME** command line in the results and history command blocks would closely parallel the pattern we see for management of the restart file names.

For the first run in our restart sequence, we will have only a **RESTART DATA** command block in the region; there will be no restart-related command line in the domain scope of our input file. We will, however, have a

```
START TIME = 0.0
```

command line in a **TIME STEPPING** command block (within the **TIME CONTROL** command block)
and a

\begin{verbatim}
TERMINATION TIME = 2.5E-3
\end{verbatim}

command line within the \texttt{TIME CONTROL} command block to set the limits for the begin and end times. The \texttt{RESTART DATA} command block in our input file will be as follows:

\begin{verbatim}
BEGIN RESTART DATA PRESTO_RESTART
 OUTPUT DATABASE NAME = RS1.rsout
 AT TIME 0.0 INCREMENT = 0.5E-3
 END RESTART DATA PRESTO_RESTART
\end{verbatim}

For our first run, the restart option will generate the following restart files:

\begin{verbatim}
RS1.rsout.2.0
RS1.rsout.2.1
\end{verbatim}

For the above files, the extensions on the file names indicate that we have a two-processor run. The 2.0 and 2.1 extensions associate the restart files with the corresponding individual mesh files on each processor. If our mesh file is \texttt{mesh.g}, then our mesh files on the individual processors will be \texttt{mesh.g.2.0} and \texttt{mesh.g.2.1}. All restart information in the above files appears at time intervals of $0.5 \times 10^{-3}$, and the last restart information is written at time $2.5 \times 10^{-3}$.

For the second run in our sequence of restart runs, we want to start at the previous termination time, $2.5 \times 10^{-3}$, and terminate at time $5.0 \times 10^{-3}$. To do this, we must add a

\begin{verbatim}
RESTART TIME = 2.5E-3
\end{verbatim}

command line to the domain scope and set the termination time to $5.0 \times 10^{-3}$ by using the command line

\begin{verbatim}
TERMINATION TIME = 5.0E-3 \rm
\end{verbatim}

within the \texttt{TIME CONTROL} command block.

It is important to note here that the actual start time for the second run in our analysis is now set by the restart time set on the \texttt{RESTART TIME} command line, $2.5 \times 10^{-3}$. The command line \texttt{START TIME = 0.0} in the \texttt{TIME STEPPING} command block is now superseded as the actual starting time for the second run by the restart commands. Any \texttt{START TIME} command line in a \texttt{TIME STEPPING} command block is still valid in terms of defining time stepping blocks (these blocks being used to set activation periods), but the restart process sets the actual start time for our analysis. This pattern of control for setting the actual start time holds for any run in our sequence of restart runs.

We also must change the \texttt{RESTART DATA} command block to the following:

\begin{verbatim}
BEGIN RESTART DATA PRESTO_RESTART
 INPUT DATABASE NAME = RS1.rsout
 OUTPUT DATABASE NAME = RS2.rsout
 AT TIME 0.0 INCREMENT = 0.5E-3
 END RESTART DATA PRESTO_RESTART
\end{verbatim}
For this second run, we will read from the following files:

- RS1.rsout.2.0
- RS1.rsout.2.1

And we will write to the following files:

- RS2.rsout.2.0
- RS2.rsout.2.1

All restart information in the above output files, RS2.rsout.2.0 and RS2.rsout.2.1, appears at time intervals of \( 0.5 \times 10^{-3} \), restart information is written from time \( 2.5 \times 10^{-3} \) to time \( 5.0 \times 10^{-3} \), and the last restart information is written at time \( 5.0 \times 10^{-3} \). Notice that we have preserved the restart files from the first run from our restart sequence of runs because we have specifically given the input and output databases distinct names—RS2.rsout for the input file name and RS1.rsout for the output file name.

Now, we want to do a third run in our sequence of restart runs. For this third run, we want to start at time \( 4.5 \times 10^{-3} \) and terminate at time \( 8.5 \times 10^{-3} \). We do not want to start at the termination time for the previous restart, which is \( 5.0 \times 10^{-3} \); rather, we want to start at time \( 4.5 \times 10^{-3} \). We change the `RESTART TIME` command line to

```
RESTART TIME = 4.5E-3
```

and the `TERMINATION TIME` command line within the `TIME CONTROL` command block to:

```
TERMINATION TIME = 8.5E-3
```

And we change the `RESTART DATA` command block to the following:

```
BEGIN RESTART DATA PRESTO_RESTART
  INPUT DATABASE NAME = RS2.rsout
  OUTPUT DATABASE NAME = RS3.rsout
  AT TIME 0.0, INCREMENT = 0.5E-3
END RESTART DATA PRESTO_RESTART
```

For this third run, we will read from the following files:

- RS2.rsout.2.0
- RS2.rsout.2.1

And we will write to the following files:

- RS3.rsout.2.0
- RS3.rsout.2.1

All restart information in the above output files, RS3.rsout.2.0 and RS3.rsout.2.1, appears at time intervals of \( 0.5 \times 10^{-3} \), restart information is written from time \( 4.5 \times 10^{-3} \) to time \( 8.5 \times 10^{-3} \), and the last restart information is written at time \( 8.5 \times 10^{-3} \). Notice that we have preserved all restart files from previous runs in our restart sequence of runs because we have specifically given the input and output databases distinct names for this third run.
8.4. RESTART DATA

8.4.1.3 Overwriting Restart Files

If you use the `RESTART TIME` command line in conjunction with the `DATABASE NAME` command line, you will overwrite restart information (unless you have included an `OVERWRITE` command line set to `ON`). As indicated previously, you will probably want to have a restart file (or files in the case of parallel runs) associated with each run in a sequence of restart runs. The example in this section shows how to overwrite restart files if that is an acceptable approach for a particular analysis.

For our first run, we will set a termination time of $1.0 \times 10^{-3}$ with the command line

```
TERMINATION TIME = 1.0E-3
```

and set the `RESTART DATA` command block as follows:

```
BEGIN RESTART DATA
  DATABASE NAME = RS.out
  AT TIME 0.0 INTERVAL = 0.25E-3
END RESTART DATA
```

Our first run will generate the following restart files:

```
RS.out.2.0
RS.out.2.1
```

All restart information in the above output files, `RS.out.2.0` and `RS.out.2.1`, appears at time intervals of $0.25 \times 10^{-3}$, restart information is written from time 0.0 to time $1.0 \times 10^{-3}$, and the last restart information is written at time $1.0 \times 10^{-3}$.

Suppose for our second run we set the termination time to $2.0 \times 10^{-3}$ with the command line

```
TERMINATION TIME = 2.0E-3
```

and add the command line

```
RESTART TIME = 1.0E-3
```

to the domain scope. We leave the `RESTART DATA` command block unchanged.

For our second run, restart information is read from the files `RS.out.2.0` and `RS.out.2.1`. These files are then overwritten with new restart information beginning at time $1.0 \times 10^{-3}$. The files `RS.out.2.0` and `RS.out.2.1` will have restart information beginning at time $1.0 \times 10^{-3}$ in intervals of $0.25 \times 10^{-3}$. The restart information will terminate at time $2.0 \times 10^{-3}$.

Now we want to do a third run with a termination time of $3.0 \times 10^{-3}$. We change the termination time by using the command line:

```
TERMINATION TIME = 3.0E-3
```

And we change the `RESTART TIME` command line so that it is now:

```
RESTART TIME = 3.0E-3
```
For our third run, restart information is read from the files \texttt{RS.out.2.0} and \texttt{RS.out.2.1}. These files are then overwritten with new restart information beginning at time $2.0 \times 10^{-3}$. The files \texttt{RS.out.2.0} and \texttt{RS.out.2.1} will have restart information beginning at time $2.0 \times 10^{-3}$ in intervals of $0.25 \times 10^{-3}$. The restart information will terminate at time $3.0 \times 10^{-3}$.

### 8.4.1.4 Recovering from a Corrupted Restart

Suppose you are using the automated option for restart and a system crash occurs when the restart file is being written. The restart file contains a corrupted entry for one of the restart times. In this case, you can continue using the automated option for restart. Restart will detect the corrupted entry and then find an entry previous to the corrupted entry that can be used for restart. This previous entry should be the entry prior to the corrupted entry unless something unusual has occurred. If the first intact restart entry is not the previous entry, restart continues to back up until an intact restart entry is found.

You could do a manual recovery. The manual recovery requires the use of a \texttt{RESTART TIME} command line to select some intact restart entry. You will have to use the \texttt{INPUT DATABASE NAME} and \texttt{OUTPUT DATABASE NAME} command lines to avoid overwriting previous restart files (see Section 8.4.1.2). You will also have to change file names in the results and history command blocks to avoid overwriting previous results and history files. Once you have done the manual recovery, you could then revert to the automatic restart option.

### 8.4.2 Overwrite Command in Restart

\[
\text{OVERWRITE} = \text{<string>}\text{OFF|ON|TRUE|FALSE|YES|NO} \quad (\text{ON|TRUE|YES})
\]

The \texttt{OVERWRITE} command line can be used to prevent the overwriting of existing restart files. The use of the automatic read and write option for restart files as described in Section 8.4.1.1 does not require the \texttt{OVERWRITE} command line. The automatic read and write option adds extensions to file names and prevents the overwriting of any existing restart files. For the case of a user-controlled read and write of restart files (Section 8.4.1.2), however, the \texttt{OVERWRITE} command line is useful for preventing the overwriting of restart files. If the \texttt{OVERWRITE} command line is set to \texttt{OFF}, \texttt{FALSE}, or \texttt{NO}, then existing restart files will not be overwritten. Execution of the code will terminate before existing restart files are overwritten. The default option is to overwrite existing restart files. If the \texttt{OVERWRITE} command line is not included, or the command line is set to \texttt{ON}, \texttt{TRUE}, or \texttt{YES}, then existing files can be overwritten.

### 8.4.3 Set Begin Time for Restart Writes

\[
\text{START TIME} = \text{<real>}\text{restart_start_time}
\]

Using the \texttt{START TIME} command line, you can write restarts to the restart file beginning at time \texttt{restart_start_time}. No restarts will be written before this time. If other commands set times
for restarts (AT TIME, ADDITIONAL TIMES) that are less than restart_start_time, those times will be ignored, and restarts will not be written at those times.

8.4.4 Adjust Interval for Time Steps

TIMESTEP ADJUSTMENT INTERVAL = <integer>steps

This command line is used to specify that the restarts will be written at exactly the times specified. To hit the restart times exactly in an explicit transient dynamics code, it is necessary to adjust the time step as the time approaches a restart time. The integer value steps in the TIMESTEP ADJUSTMENT INTERVAL command line specifies the number of time steps to look ahead in order to adjust the time step.

If this command line does not appear, then restarts are written at times closest to the specified restart times.

8.4.5 Restart Interval Specified by Time Increment

AT TIME <real>time_begin INCREMENT = <real>time_increment Dt

At the time specified by time_begin, restarts will be written every time increment given by the real value time_incrementDt.

8.4.6 Additional Times for Restart

ADDITIONAL TIMES = <real>output_time1 <real>output_time2 ...

In addition to any restart times specified by the command line in Section 8.4.5, you can use the ADDITIONAL TIMES command line to specify an arbitrary number of additional restart times.

8.4.7 Restart Interval Specified by Step Increment

AT STEP <integer>step_begin INCREMENT =
<integer>step_increment

At the step specified by step_begin, restarts will be written every step increment given by the integer value step_increment.
8.4.8 Additional Steps for Restart

ADDITIONAL STEPS = <integer>output_step1
<integer>output_step2 ...

In addition to any steps specified by the command line in Section 8.4.7, you can use the ADDITIONAL STEPS command line to specify an arbitrary number of additional restart steps.

8.4.9 Set End Time for Restart Writes

TERMINATION TIME = <real>termination_time_value

Restarts will not be written to the restart file after time termination_time_value. If other commands set times for restarts (AT TIME, ADDITIONAL TIMES) that are greater than termination_time_value, those times will be ignored, and restarts will not be written at those times.

8.4.10 Overlay Count

OVERLAY COUNT = <integer>overlay_count

The OVERLAY COUNT command line specifies the number of restart output times that will be overlaid on top of the current step before advancing to the next step. For example, suppose that we set the overlay_count parameter to 2, and we request that restart information be written every 0.1 second. At time 0.1 second, restart step 1 will be written to the output restart database. At time 0.2 second, restart information will be written over the step 1 information, which originally contained restart information at 0.1 second. At time 0.3 second, restart information will be written over the step 1 information, which last contained information at 0.2 second. At time 0.4 second, we will now write step 2 to the output restart database (step 1 has already been written over twice). At time 0.5 second, restart information will be written over the step 2 information, which originally contained information at 0.4 second. At time 0.6 second, restart information will be written over the step 2 information, which last contained information at 0.5 second. At time 0.7 second, restart step 3 will be written to the output restart database (step 2 has already been written over twice). This pattern continues so that we would build up a sequence of restart information at times 0.3, 0.6, 0.9, . . . second until we reach the termination time for the problem. If there was a problem during the analysis, the last step on the output restart database would be whatever last had been written to the database. If, for example, we had set our termination time to 1.0 second and a problem occurred after restart information had been written at 0.7 second but before we completed the time step at 0.8 second, then the last information on the output restart database would be at 0.7 second.

You can use the OVERLAY COUNT command line in conjunction with a CYCLE COUNT command line. For a description of the CYCLE COUNT command line and its use with the OVERLAY COUNT command line, see Section 8.4.11.
8.4.11 Cycle Count

CYCLE COUNT = <integer>cycle_count

The CYCLE COUNT command line specifies the number of restart steps that will be written to the output restart database before previously written steps are overwritten. For example, suppose we set the cycle_count parameter to 5, and we request that restart information be written every 0.1 second. The restart system will write information to the output restart database at times 0.1, 0.2, 0.3, 0.4, and 0.5 second. At time 0.6 second, the information at step 1, originally written at time 0.1 second, will be overwritten with information at time 0.6 second. At time 0.7 second, the information at step 2, originally written at time 0.2 second, will be overwritten with information at time 0.7 second. At time 0.8 second, the output restart database will contain restart information at times 0.6, 0.7, 0.8, 0.4, and 0.5 second. Time will not necessarily be monotonically increasing on a database that uses a CYCLE COUNT command line.

If you only want the last step available on the output restart database, set cycle_count equal to 1.

The CYCLE COUNT and OVERLAY COUNT command lines can be used at the same time. For this example, we will combine our example with an overlay count of 2 as given in Section 8.4.10 with our example of a cycle count of 5 as given in this section (Section 8.4.11). Information is written to the output restart database time step every 0.1 second. The output times at which information is written to the output restart database are 0.1, 0.2, 0.3, . . . second. Each of these times corresponds to an output step. Time 0.1 second corresponds to output step 1, time 0.2 second corresponds to output step 2, time 0.3 corresponds to output step 3, and so forth. An output time of \( n \times 0.1 \) corresponds to output step \( n \). The overlay command will result in information at time 0.3, 0.6, 0.9, 1.2, and 1.5 seconds written as steps 1, 2, 3, 4, and 5 on the output restart database. For times greater than 1.6 seconds, the cycle command will now take effect because we have five steps written on the output restart database. Information at times 1.6, 1.7, and 1.8 seconds will now overwrite the information at step 1, which had information at time 0.3 second. Information at times 1.9, 2.0, and 2.1 seconds will now overwrite the information at step 2, which had information at time 0.6 second. For any output step \( n \), its position, step number \( n_s \), in the restart output database is as follows:

\[
\text{if } n_s \neq 0 \\
\quad n_s = \text{int}(n/(n_o + 1))\%n_c \\
\text{else} \\
\quad n_s = n_c \\
\end{align*}

In the above equations, \( n_c \) is the cycle count, and \( n_o \) is the overlay count. The expression \( \text{int}(n/(n_o + 1)) \) produces an integer arithmetic result. For example, if \( n \) is 4 and \( n_o \) is 2, then we have 4 divided by 3, and the integer arithmetic result is 1 (any fractional remainder is discarded). The operator \( \% \) is the modulus operator; the modulus operator gives the modulus of its first operand with respect
to its second operand, i.e., it produces the remainder of dividing the first operand by the second operand. The result of \( 1 \% 5 \) is 1, for example.

### 8.4.12 Use Output Scheduler

```
USE OUTPUT SCHEDULER <string>scheduler_name
```

In an analysis with multiple regions, it can be difficult to synchronize output such as restart files. To help synchronize output for analyses with multiple regions, you can define an `OUTPUT SCHEDULER` command block at the domain level. The scheduler can then be referenced in the `RESTART DATA` command block via the `USE OUTPUT SCHEDULER` command line. The string `scheduler_name` must match a name used in an `RESTART DATA` command block. See Section 8.5 for a description of using this command block and the `USE OUTPUT SCHEDULER` command line.

### 8.4.13 Write Restart If System Error Encountered

```
OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
                   SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
                   SIGKILL|SIGILL|SIGSEGV
```

The `OUTPUT ON SIGNAL` command line is used to initiate the writing of a restart file when the system encounters a type of system error. Only one error type in the list of error types should be entered for this command line. Generally, these system errors cause the code to terminate before the code can add any current restart output (restart output past the last restart output time step) to the restart file. If the code encounters the specified type of error during execution, a restart file will be written before execution is terminated.

This command line can also be used to force the writing of a restart file at some point during execution of the code. Suppose the command line

```
OUTPUT ON SIGNAL = SIGUSR2
```

is included in the input file. While the code is running, a user can execute (from the keyboard) the system command line

```
kill -s SIGUSR2 pid
```

to terminate execution and force the writing of a results file. In the above system command line, `pid` is the process identifier, which is an integer.

The most useful application of the command line is to send a signal via a system command line to write a restart file. Note that the `OUTPUT ON SIGNAL` command line is primarily a debugging tool for code developers.
8.5 Output Scheduler

In an analysis with multiple regions, it can be difficult to synchronize output such as results files, history files, and restart files. To help synchronize output for analyses with multiple regions, you can define an OUTPUT SCHEDULER command block at the domain level. This scheduler can then be referenced in several places:

- The scheduler can be referenced in the RESULTS OUTPUT command block to control the output of results information.
- The scheduler can be referenced in the HISTORY OUTPUT command block to control the output of history information.
- The scheduler can be referenced in the RESTART DATA command block to control the writing of restart files.

In summary, the OUTPUT SCHEDULER command block is defined in the domain scope. The scheduler is referenced by a USE OUTPUT SCHEDULER command line that can appear in a RESULTS OUTPUT, HISTORY OUTPUT, and RESTART DATA command block. Section 8.5.1 describes the OUTPUT SCHEDULER command block, and Section 8.5.2 illustrates how this block is referenced with the USE OUTPUT SCHEDULER command line.

8.5.1 Output Scheduler Command Block

BEGIN OUTPUT SCHEDULER <string>scheduler_name
START TIME = <real>output_start_time
TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
AT TIME <real>time_begin INCREMENT =
<real>time_increment_dt
ADDITIONAL TIMES = <real>output_time1 <real>output_time2 ...
AT STEP <integer>step_begin INCREMENT =
<integer>step_increment
ADDITIONAL STEPS = <integer>output_step1 <integer>output_step2 ...
TERMINATION TIME = <real>termination_time_value
END [OUTPUT SCHEDULER <string>scheduler_name]

An output scheduler is defined with a command block in the domain scope. The OUTPUT SCHEDULER command block begins with the input line:

BEGIN OUTPUT SCHEDULER <string>scheduler_name

and is terminated with the line:

END OUTPUT SCHEDULER <string>scheduler_name
where scheduler_name is a user-defined name for the command block. All the normal scheduling command lines are valid in an OUTPUT SCHEDULER command block.

8.5.1.1 Set Begin Time for Output Scheduler

\[ \text{START TIME} = \text{<real>output_start_time} \]

Using the START TIME command line, you can set the start time for a scheduler beginning at time \( \text{output_start_time} \). The scheduler will not take effect before this time. If other commands set times for scheduling (AT TIME, ADDITIONAL TIMES) that are less than \( \text{output_start_time} \), those times will be ignored.

8.5.1.2 Adjust Interval for Time Steps

\[ \text{TIMESTEP ADJUSTMENT INTERVAL} = \text{<integer>steps} \]

This command line is used to specify that, when the scheduler is in effect, output will be at exactly the times specified. To hit the output times exactly in an explicit, transient dynamics code, it is necessary to adjust the time step as the time approaches an output time. The integer value \( \text{steps} \) in the TIMESTEP ADJUSTMENT INTERVAL command line specifies the number of time steps to look ahead in order to adjust the time step.

If this command line does not appear, output occurs at times closest to the specified output times.

8.5.1.3 Output Interval Specified by Time Increment

\[ \text{AT TIME} \quad \text{<real>time_begin} \quad \text{INCREMENT} = \quad \text{<real>time_increment_dt} \]

At the time specified by \( \text{time_begin} \), output will be scheduled at every time increment given by the real value \( \text{time_increment_dt} \).

8.5.1.4 Additional Times for Output

\[ \text{ADDITIONAL TIMES} = \quad \text{<real>output_time1} \quad \text{<real>output_time2} \ldots \]

In addition to any times specified by the command line in Section 8.5.1.3, you can use the ADDITIONAL TIMES command line to specify an arbitrary number of additional output times.

8.5.1.5 Output Interval Specified by Step Increment

\[ \text{AT STEP} \quad \text{<integer>step_begin} \quad \text{INCREMENT} = \quad \text{<integer>step_increment} \]
At the step specified by `step_begin`, output will be scheduled at every step increment given by the integer value `step_increment`.

### 8.5.1.6 Additional Steps for Output

```
ADDITIONAL STEPS = <integer>output_step1 <integer>output_step2 ...
```

In addition to any steps specified by the command line in Section 8.5.1.5, you can use the `ADDITIONAL STEPS` command line to specify an arbitrary number of additional output steps.

### 8.5.1.7 Set End Time for Output Scheduler

```
TERMINATION TIME = <real>termination_time_value
```

Using the `TERMINATION TIME` command line, you can set the termination time for a scheduler beginning at time `termination_time_value`. The scheduler will not be in effect after this time. If other commands set times for scheduling (AT TIME, ADDITIONAL TIMES) that are greater than `termination_time_value`, those times will be ignored by the scheduler.

### 8.5.2 Example of Using the Output Scheduler

Once an output scheduler has been defined via the `OUTPUT SCHEDULER` command block, it can be used by inserting a `USE OUTPUT SCHEDULER` command line in any of the following command blocks: RESULTS OUTPUT, HISTORY OUTPUT, and RESTART DATA. The following paragraph provides an example of using output schedulers.

In the domain scope, we define two output schedulers, `Timer` and `Every_Step`:

```
BEGIN OUTPUT SCHEDULER Timer
  AT TIME 0.0 INCREMENT = 10.0e-6
  TIME STEP ADJUSTMENT INTERVAL = 4
END OUTPUT SCHEDULER Timer

# BEGIN OUTPUT SCHEDULER Every_Step
BEGIN OUTPUT SCHEDULER Every_Step
  AT STEP 0 INCREMENT = 1
END OUTPUT SCHEDULER Every_Step
```

With the `USE OUTPUT SCHEDULER` command, we reference the scheduler named `Timer` for results output:

```
BEGIN RESULTS OUTPUT Out_Region_1
```

USE OUTPUT SCHEDULER Timer
.
END RESULTS OUTPUT Out_Region_1

With the USE OUTPUT SCHEDULER command, we reference the scheduler named Every_STEP for history output:

BEGIN HISTORY OUTPUT Out_Region_2
  USE OUTPUT SCHEDULER Every_Step
.
END HISTORY OUTPUT Out_Region_2
8.6 Registered Variables

This section lists commonly used registered variables that the user can select as output to the results file and the history file. The first part of this section lists global, nodal, and element registered variables. The second part of this section lists registered variables associated with material models.

8.6.1 Global, Nodal, and Element Registered Variables

This section lists commonly used global, nodal, and element registered variables. The registered variables are presented in tables based on use, as follows:

- Table 8.5 Variables Registered on Nodes (Variable and Type)
- Table 8.6 Element Variables Registered for All Elements
- Table 8.7 Element Variables Registered for Energy-Dependent (“Equation-of-State”) Elements
- Table 8.8 Element Variables Registered for Solid Elements
- Table 8.9 Element Variables Registered for Membranes
- Table 8.10 Nodal Variables Registered for Shells
- Table 8.11 Element Variables Registered for Shells
- Table 8.12 Element Variables Registered for Truss
- Table 8.13 Element Variables Registered for Beam
- Table 8.14 Element Variables Registered for Springs
- Table 8.15 Global Registered Variables
- Table 8.16 Nodal Variables Registered for Spot Welds

The tables provide the following information about each registered variable:

**Variable Name.** This is the string that will appear on the GLOBAL VARIABLES, NODE VARIABLES, or ELEMENT VARIABLES command line.

**Type.** This is the variable’s type. The various types are denoted with the labels Integer, Real, Vector_2D, Vector_3D, SymTen33, and FullTen36. The type Integer indicates the registered variable is an integer; the type Real indicates the registered variable is a real. The type Vector_2D indicates the registered variable type is a two-dimensional vector. The type Vector_3D indicates the registered variable is a three-dimensional vector. For a three-dimensional vector, the variable quantities will be output with suffixes of _x, _y, and _z. For example, if the registered variable displacement is requested to be output as displ, the components of the
displacement vector on the results file will be \text{displ}_x, \text{displ}_y, \text{and} \text{displ}_z. The type \text{SymTen33} indicates the registered variable is a symmetric $3 \times 3$ tensor. For a $3 \times 3$ symmetric tensor, the variable quantities will be output with suffixes of \_xx, \_yy, \_zz, \_xy, \_yz, \text{and} \_zx. For example, if the registered variable \text{rotated\_stress} is requested for output as \text{stress}, the components of the stress tensor on the results file will be \text{stress}_xx, \text{stress}_yy, \text{stress}_zz, \text{stress}_xy, \text{stress}_yz, \text{and} \text{stress}_zx. The type \text{FullTen36} is a full $3 \times 3$ tensor with three diagonal terms and six off-diagonal terms.

The tables of registered variables follow.

### Table 8.5: Variables Registered on Nodes (Variable and Type)

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Type</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>\text{model_coordinates}</td>
<td>\text{Vector_3D}</td>
<td>Original coordinates of nodes.</td>
</tr>
<tr>
<td>\text{coordinates}</td>
<td>\text{Vector_3D}</td>
<td>Current coordinates of nodes.</td>
</tr>
<tr>
<td>\text{displacement}</td>
<td>\text{Vector_3D}</td>
<td>Total displacement.</td>
</tr>
<tr>
<td>\text{displacement_increment}</td>
<td>\text{Vector_3D}</td>
<td>Displacement increment at current time step.</td>
</tr>
<tr>
<td>\text{velocity}</td>
<td>\text{Vector_3D}</td>
<td></td>
</tr>
<tr>
<td>\text{acceleration}</td>
<td>\text{Vector_3D}</td>
<td></td>
</tr>
<tr>
<td>\text{force_internal}</td>
<td>\text{Vector_3D}</td>
<td></td>
</tr>
<tr>
<td>\text{force_external}</td>
<td>\text{Vector_3D}</td>
<td></td>
</tr>
<tr>
<td>\text{force_hourglass}</td>
<td>\text{Vector_3D}</td>
<td></td>
</tr>
<tr>
<td>\text{force_contact}</td>
<td>\text{Vector_3D}</td>
<td></td>
</tr>
<tr>
<td>\text{reactions}</td>
<td>\text{Vector_3D}</td>
<td></td>
</tr>
<tr>
<td>\text{moment_reactions}</td>
<td>\text{Vector_3D}</td>
<td></td>
</tr>
<tr>
<td>\text{mass}</td>
<td>\text{Real}</td>
<td></td>
</tr>
</tbody>
</table>

### Table 8.6: Element Variables Registered for All Elements

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Type</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>\text{elem_time_step}</td>
<td>\text{Real}</td>
<td>Critical time step for the element. The element in the model with the smallest time step controls the analysis time step.</td>
</tr>
<tr>
<td>\text{element_mass}</td>
<td>\text{Real}</td>
<td></td>
</tr>
</tbody>
</table>
### Table 8.7: Element Variables Registered for Energy-Dependent (“Equation-of-State”) Elements

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Type</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>stress</td>
<td>SymTen33</td>
<td></td>
</tr>
<tr>
<td>rotated_stress</td>
<td>SymTen33</td>
<td></td>
</tr>
<tr>
<td>stretch</td>
<td>SymTen33</td>
<td></td>
</tr>
<tr>
<td>rotation</td>
<td>FullTen36</td>
<td></td>
</tr>
<tr>
<td>element_density</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>sound_speed</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>specific_internal_energy</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>artificial_viscosity</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>volume</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>shrmod</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>dilmod</td>
<td>Real</td>
<td></td>
</tr>
</tbody>
</table>

### Table 8.8: Element Variables Registered for Solid Elements

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Type</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>stress</td>
<td>SymTen33</td>
<td></td>
</tr>
<tr>
<td>rotated_stress</td>
<td>SymTen33</td>
<td></td>
</tr>
<tr>
<td>stretch</td>
<td>SymTen33</td>
<td></td>
</tr>
<tr>
<td>rotation</td>
<td>FullTen36</td>
<td></td>
</tr>
<tr>
<td>log_strain</td>
<td>SymTen33</td>
<td></td>
</tr>
<tr>
<td>volume</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>shrmod</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>dilmod</td>
<td>Real</td>
<td></td>
</tr>
</tbody>
</table>

### Table 8.9: Element Variables Registered for Membranes

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Type</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>memb_stress</td>
<td>SymTen33</td>
<td></td>
</tr>
<tr>
<td>element_area</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>element_thickness</td>
<td>Real</td>
<td></td>
</tr>
</tbody>
</table>
Table 8.10: Nodal Variables Registered for Shells

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Type</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>rotational_displacement</td>
<td>Vector_3D</td>
<td></td>
</tr>
<tr>
<td>rotational_velocity</td>
<td>Vector_3D</td>
<td></td>
</tr>
<tr>
<td>rotational_acceleration</td>
<td>Vector_3D</td>
<td></td>
</tr>
<tr>
<td>moment_internal</td>
<td>Vector_3D</td>
<td></td>
</tr>
<tr>
<td>moment_external</td>
<td>Vector_3D</td>
<td></td>
</tr>
<tr>
<td>rotational_mass</td>
<td>Real</td>
<td></td>
</tr>
</tbody>
</table>

Table 8.11: Element Variables Registered for Shells

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Type</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>memb_stress</td>
<td>SymTen33</td>
<td>Stress at midplane in global X, Y, and Z coordinates.</td>
</tr>
<tr>
<td>bottom_stress</td>
<td>SymTen33</td>
<td>Stress at bottom integration point in global X, Y, and Z coordinates.</td>
</tr>
<tr>
<td>top_stress</td>
<td>SymTen33</td>
<td>Stress at top integration point in global X, Y, and Z coordinates.</td>
</tr>
<tr>
<td>strain</td>
<td>SymTen33</td>
<td>Integrated strain at midplane in local shell coordinate system.</td>
</tr>
<tr>
<td>element_area</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>element_thickness</td>
<td>Real</td>
<td></td>
</tr>
</tbody>
</table>

Table 8.12: Element Variables Registered for Truss

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Type</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>truss_init_length</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>truss_stretch</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>truss_stress</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>truss_strain_incr</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>truss_force</td>
<td>Real</td>
<td></td>
</tr>
</tbody>
</table>
### Table 8.13: Element Variables Registered for Beam

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Type</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>beam_strain_inc</td>
<td>Vector_2D</td>
<td>Thirty-two strain increment values are output. Some values may be zero depending on section. Axial strains are 01, 03, 05, . . . Shear strains are 02, 04, 06, . . . See Section 5.2.4 for more details.</td>
</tr>
<tr>
<td>beam_stress</td>
<td>Vector_2D</td>
<td>Thirty-two stress values are output. Some values may be zero depending on section. Axial stresses are 01, 03, 05, . . . Shear stresses are 02, 04, 06, . . . See Section 5.2.4 for more details.</td>
</tr>
<tr>
<td>beam_stress_axial</td>
<td>Real</td>
<td>Sixteen axial stress values. Some may be zero depending on section.</td>
</tr>
<tr>
<td>beam_stress_shear</td>
<td>Real</td>
<td>Sixteen shear stress values. Some may be zero depending on section.</td>
</tr>
<tr>
<td>beam_axial_force</td>
<td>Real</td>
<td>Axial force at midpoint.</td>
</tr>
<tr>
<td>beam_transverse_force_s</td>
<td>Real</td>
<td>Transverse shear in s-direction at midpoint.</td>
</tr>
<tr>
<td>beam_transverse_force_t</td>
<td>Real</td>
<td>Transverse shear in t-direction at midpoint.</td>
</tr>
<tr>
<td>beam_moment_r</td>
<td>Real</td>
<td>Torsion at midpoint.</td>
</tr>
<tr>
<td>beam_moment_s</td>
<td>Real</td>
<td>Moment about s-direction at midpoint.</td>
</tr>
<tr>
<td>beam_moment_t</td>
<td>Real</td>
<td>Moment about t-direction at midpoint.</td>
</tr>
</tbody>
</table>

### Table 8.14: Element Variables Registered for Springs

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Type</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>spring_force</td>
<td>Real</td>
<td>Magnitude of the internal spring force.</td>
</tr>
<tr>
<td>spring_engineering_strain</td>
<td>Real</td>
<td>Change in length over initial length $\frac{dL}{L_0}$.</td>
</tr>
<tr>
<td>spring_init_length</td>
<td>Real</td>
<td>Initial spring length, $L_0$.</td>
</tr>
</tbody>
</table>

### Table 8.15: Global Registered Variables

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Type</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>timestep</td>
<td>Real</td>
<td></td>
</tr>
<tr>
<td>KineticEnergy</td>
<td>Real</td>
<td>Momentum in global X-direction.</td>
</tr>
<tr>
<td>MomentumX</td>
<td>Real</td>
<td>Momentum in global Y-direction.</td>
</tr>
<tr>
<td>MomentumY</td>
<td>Real</td>
<td>Momentum in global Z-direction.</td>
</tr>
<tr>
<td>MomentumZ</td>
<td>Real</td>
<td></td>
</tr>
</tbody>
</table>
Table 8.16: Nodal Variables Registered for Spot Welds

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Type</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>SPOT_WELD%parametric_coords</td>
<td>Vector_2D</td>
<td>Coordinates of node on face.</td>
</tr>
<tr>
<td>SPOT_WELD%norm_force_at_death</td>
<td>Real</td>
<td>Value of force normal to face when spot-weld breaks.</td>
</tr>
<tr>
<td>SPOT_WELD%tang_force_at_death</td>
<td>Real</td>
<td>Value of force tangential to face when spot-weld breaks.</td>
</tr>
<tr>
<td>SPOT_WELD%death_flag</td>
<td>Integer</td>
<td>alive = 0, dead = FAILURE DECAY CYCLES (default is 10).</td>
</tr>
<tr>
<td>SPOT_WELD%scale_factor</td>
<td>Real</td>
<td>Nodal influence area of current node.</td>
</tr>
<tr>
<td>SPOT_WELD%norm_displacement</td>
<td>Real</td>
<td>Current displacement of weld normal to face.</td>
</tr>
<tr>
<td>SPOT_WELD%tang_displacement</td>
<td>Real</td>
<td>Current displacement of weld tangential to face.</td>
</tr>
<tr>
<td>SPOT_WELD%norm_force</td>
<td>Real</td>
<td>Current force of weld normal to face.</td>
</tr>
<tr>
<td>SPOT_WELD%tang_force</td>
<td>Real</td>
<td>Current force of weld tangential to face.</td>
</tr>
<tr>
<td>SPOT_WELD%initial_offset</td>
<td>Vector_3D</td>
<td>The initial offset of the spot weld node from the spot weld surface. Does not change over time, only output if IGNORE INITIAL OFFSET = YES is specified at input.</td>
</tr>
<tr>
<td>SPOT_WELD%initial_normal</td>
<td>Vector_3D</td>
<td>The initial normal of the spot weld surface at the point of interaction. Only output if IGNORE INITIAL OFFSET = YES is specified at input.</td>
</tr>
</tbody>
</table>
8.6. REGISTERED VARIABLES

8.6.2 Registered Variables for Material Models

It is possible to output the state variables from the material models. Most of the materials, with the exception of simple models such as the elastic model, have state variables that can be output. The method used to output state variables depends on how the model is implemented. There are currently three cases:

- The native version of most of the solid models for which state variables are accessed by index
- The native version of a few solid models for which state variables are accessed by name
- The versions of the solid models implemented in the LAME library for which state variables are accessed by name

In the future, the implementation of the solid material models in LAME will be used by default, and all state variables will be accessed by name. The following sections describe the different methods required to output material model variables.

8.6.2.1 State Variable Output by Index for Native Solid Material Models

There are two ways to output the state variables for the native material models. The simplest way outputs all of the state variables for a given material model. Use the `ELEMENT VARIABLES` command line in the `RESULTS OUTPUT` command block of the form:

```
ELEMENT VARIABLES = state_material_name
```

where `material_name` is the name of the material model, e.g. `elastic_plastic`, `power_law_hardening`, `foam_plasticity`, or `orthotropic_rate`. All of the state variables for the material will be output.

If it is desired to output a subset of the state variables for a material model, one must use a different syntax in which the variable name starts with `MAT%`. This `MAT%` syntax allows for all or part of the state variables for a material to be output. In this case, the `ELEMENT VARIABLES` command line in the `RESULTS OUTPUT` command block has the following form:

```
ELEMENT VARIABLES = MAT%material_name
```

where `material_name` is the name of the material model, e.g. `elastic_plastic`, `power_law_hardening`, `foam_plasticity`, or `orthotropic_rate`.

For example, if you wanted to get all the state variables for the elastic-plastic material model, you would use:

```
ELEMENT VARIABLES = MAT%elastic_plastic
```

or

```
ELEMENT VARIABLES = MAT%elastic_plastic(:)
```
In the preceding command line, the parentheses indicate a subset of the state variables, and the colon should be read as “through.” The notation (:) implies all the state variables; the notion (3:7) would imply state variables 3 through 7.

Depending on the material type, there may be several hundred material state variables. A subset of state variables may be output using a FORTRAN-like array syntax. For example, to output the equivalent plastic strain for the elastic-plastic material and rename it to something meaningful, use:

```
ELEMENT VARIABLES = MAT%elastic_plastic(1) as eqps
```

To output a six-entry symmetric tensor subset of the orthotropic rate material, use:

```
ELEMENT VARIABLES = MAT%orthotropic_rate(2:7)
```

Finally, if a scattered set of material variables is desired, the variables may be selected by using the \mid array operator, as in the command:

```
ELEMENT VARIABLES = MAT%foam_plasticity(1\mid 4\mid 6\mid 9)
```

This command would output state variables 1, 4, 5, 6, and 9 of the foam plasticity model.

Section 8.6.2.4 provides tables listing the state variables for all solid material models. Models for which state variable output is requested using the method described here have indices entered in a column entitled "Index (Native Model)".

8.6.2.2 State Variable Output by Name for Native Solid Material Models

Some of the native material models are implemented in a way such that state variables are accessed directly by name rather than by index. For example, to access the \textit{C10} variable in the Mooney-Rivlin material model, one would simply list the name \textit{C10} to obtain that output. The state variables for the Mooney-Rivlin, Swanson, and Orthotropic Crush material models are accessed in this way. In addition, the state variables for all of the energy-dependent models (Mie-Gruneisen, Mie-Gruneisen Power-Series, JWL, and ideal gas) are accessed this way.

Section 8.6.2.4 provides tables listing the state variables for all solid material models. Models for which state variable output is requested by name have names entered in a column entitled "Name (Native Model)".

8.6.2.3 State Variable Output for LAME Solid Material Models

The state variables for material models in LAME are accessible directly by name. For instance, the equivalent plastic strain variable is accessible by the name \textit{EQPS} for all elastic-plastic material models.

Section 8.6.2.4 provides tables listing the state variables for all solid material models. Models that are implemented in LAME have state variable names listed in the column entitled "Name (LAME Model)". If there are no entries in that column for a given material, then that material is not implemented in LAME.
8.6. REGISTERED VARIABLES

8.6.2.4 State Variable Tables for Solid Material Models

As explained in the preceding sections, there are three cases to be considered for state variable output from solid material models: native models for which state output is obtained using an index with the \texttt{MAT}\% syntax, native models for which state output is obtained using the variable name, and LAME models, for which state output is also obtained by variable name. Tables of state variables for commonly used material models are provided in Tables 8.17 through 8.42. These tables contain the indices or names used to access the state variables in the native version of the models, as well as the names used to access the LAME versions of the models. If there are no entries in the "Native Model" column for a model, that model is only implemented in LAME. Likewise, if there are no entries in the "LAME Model" column, there is no version of that model in LAME.

Table 8.17: State Variables for DUCTILE FRACTURE Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>EQPS</td>
<td>equivalent plastic strain</td>
</tr>
<tr>
<td>2</td>
<td>TEAR</td>
<td>tearing parameter</td>
</tr>
<tr>
<td>3</td>
<td>CRIT_COS</td>
<td>crack opening strain</td>
</tr>
<tr>
<td>4</td>
<td>CD_X</td>
<td>crack opening direction - x component</td>
</tr>
<tr>
<td>5</td>
<td>CD_Y</td>
<td>crack opening direction - y component</td>
</tr>
<tr>
<td>6</td>
<td>CD_Z</td>
<td>crack opening direction - z component</td>
</tr>
<tr>
<td>7</td>
<td>FLAG_DEATH</td>
<td>flag for element death</td>
</tr>
<tr>
<td>8</td>
<td>RADIUS</td>
<td>radius of yield surface</td>
</tr>
</tbody>
</table>

Table 8.18: State Variables for ELASTIC Model

This model has no state variables.

Table 8.19: State Variables for ELASTIC FRACTURE Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>FLAG_DEATH</td>
<td>flag for element death</td>
</tr>
<tr>
<td>2</td>
<td>CRIT_COS</td>
<td>critical value of opening strain</td>
</tr>
<tr>
<td>3</td>
<td>CD_X</td>
<td>crack opening direction - x component</td>
</tr>
<tr>
<td>4</td>
<td>CD_Y</td>
<td>crack opening direction - y component</td>
</tr>
<tr>
<td>5</td>
<td>CD_Z</td>
<td>crack opening direction - z component</td>
</tr>
<tr>
<td>6</td>
<td>MAXSTRESS</td>
<td>value of maximum principal stress</td>
</tr>
</tbody>
</table>
Table 8.20: State Variables for ELASTIC PLASTIC Model

<table>
<thead>
<tr>
<th>Index</th>
<th>Name (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>EQPS</td>
<td></td>
<td>equivalent plastic strain</td>
</tr>
<tr>
<td>2</td>
<td>ALPHA_XX</td>
<td></td>
<td>back stress - xx component</td>
</tr>
<tr>
<td>3</td>
<td>ALPHA YY</td>
<td></td>
<td>back stress - yy component</td>
</tr>
<tr>
<td>4</td>
<td>ALPHA ZZ</td>
<td></td>
<td>back stress - zz component</td>
</tr>
<tr>
<td>5</td>
<td>ALPHA_XY</td>
<td></td>
<td>back stress - xy component</td>
</tr>
<tr>
<td>6</td>
<td>ALPHA_YZ</td>
<td></td>
<td>back stress - yz component</td>
</tr>
<tr>
<td>7</td>
<td>ALPHA_ZX</td>
<td></td>
<td>back stress - zx component</td>
</tr>
<tr>
<td></td>
<td>RADIUS</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 8.21: State Variables for EP POWER HARD Model

<table>
<thead>
<tr>
<th>Index</th>
<th>Name (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>EQPS</td>
<td></td>
<td>equivalent plastic strain</td>
</tr>
<tr>
<td>2</td>
<td>RADIUS</td>
<td></td>
<td>radius of yield surface</td>
</tr>
</tbody>
</table>

Table 8.22: State Variables for FOAM PLASTICITY Model

<table>
<thead>
<tr>
<th>Index</th>
<th>Name (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ITER</td>
<td></td>
<td>iterations</td>
</tr>
<tr>
<td>2</td>
<td>VOL_STRAIN</td>
<td></td>
<td>volumetric strain</td>
</tr>
<tr>
<td>3</td>
<td>PHI</td>
<td></td>
<td>phi</td>
</tr>
<tr>
<td>4</td>
<td>EQPS</td>
<td></td>
<td>equivalent plastic strain</td>
</tr>
<tr>
<td>5</td>
<td>PA</td>
<td></td>
<td>A</td>
</tr>
<tr>
<td>6</td>
<td>PB</td>
<td></td>
<td>B</td>
</tr>
</tbody>
</table>

Table 8.23: State Variables for HONEYCOMB Model

<table>
<thead>
<tr>
<th>Index</th>
<th>Name (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CRUSH</td>
<td></td>
<td>minimum volume ratio</td>
</tr>
<tr>
<td>2</td>
<td>EQDOT</td>
<td></td>
<td>effective strain rate</td>
</tr>
<tr>
<td>3</td>
<td>RMULT</td>
<td></td>
<td>rate multiplier</td>
</tr>
<tr>
<td>5</td>
<td>ITER</td>
<td></td>
<td>iterations</td>
</tr>
<tr>
<td>6</td>
<td>EVOL</td>
<td></td>
<td>volumetric strain</td>
</tr>
</tbody>
</table>
### Table 8.24: State Variables for HYPERFOAM Model

This model has no state variables.

### Table 8.25: State Variables for JOHNSON COOK Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>RADIUS</td>
<td>radius of yield surface</td>
</tr>
<tr>
<td>2</td>
<td>EQPS</td>
<td>equivalent plastic strain</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>temperature</td>
</tr>
<tr>
<td>4</td>
<td>EQDOT</td>
<td>equivalent strain rate</td>
</tr>
<tr>
<td>5</td>
<td></td>
<td>iterations</td>
</tr>
</tbody>
</table>

### Table 8.26: State Variables for LOW DENSITY FOAM Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>PAIR</td>
<td></td>
</tr>
</tbody>
</table>
Table 8.27: State Variables for MOONEY RIVLIN Model

<table>
<thead>
<tr>
<th>Name (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>C01</td>
<td>C01</td>
<td></td>
</tr>
<tr>
<td>C10</td>
<td>C10</td>
<td></td>
</tr>
<tr>
<td>RK</td>
<td>K</td>
<td></td>
</tr>
<tr>
<td>SFJth</td>
<td>SFJTH</td>
<td></td>
</tr>
<tr>
<td>RJTH</td>
<td>JTH</td>
<td></td>
</tr>
<tr>
<td>V_MECH</td>
<td>VMECH_XX</td>
<td></td>
</tr>
<tr>
<td></td>
<td>VMECH_YY</td>
<td></td>
</tr>
<tr>
<td></td>
<td>VMECH_ZZ</td>
<td></td>
</tr>
<tr>
<td></td>
<td>VMECH_XY</td>
<td></td>
</tr>
<tr>
<td></td>
<td>VMECH_YZ</td>
<td></td>
</tr>
<tr>
<td></td>
<td>VMECH_ZX</td>
<td></td>
</tr>
<tr>
<td></td>
<td>SFJTH_FLAG</td>
<td></td>
</tr>
</tbody>
</table>

Table 8.28: State Variables for MULTILINEAR EP Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>EQPS</td>
<td>equivalent plastic strain</td>
</tr>
<tr>
<td>2</td>
<td>RADIUS</td>
<td>radius of yield surface</td>
</tr>
<tr>
<td>3</td>
<td>ALPHA_XX</td>
<td>back stress - xx component</td>
</tr>
<tr>
<td>4</td>
<td>ALPHA_YY</td>
<td>back stress - yy component</td>
</tr>
<tr>
<td>5</td>
<td>ALPHA_ZZ</td>
<td>back stress - zz component</td>
</tr>
<tr>
<td>6</td>
<td>ALPHA_XY</td>
<td>back stress - xy component</td>
</tr>
<tr>
<td>7</td>
<td>ALPHA_YZ</td>
<td>back stress - yz component</td>
</tr>
<tr>
<td>8</td>
<td>ALPHA_ZX</td>
<td>back stress - zx component</td>
</tr>
</tbody>
</table>
### Table 8.29: State Variables for ML EP FAIL Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>EQPS</td>
<td>equivalent plastic strain</td>
</tr>
<tr>
<td>2</td>
<td>RADIUS</td>
<td>radius of yield surface</td>
</tr>
<tr>
<td>3</td>
<td>ALPHA_XX</td>
<td>back stress - xx component</td>
</tr>
<tr>
<td>4</td>
<td>ALPHA_YY</td>
<td>back stress - yy component</td>
</tr>
<tr>
<td>5</td>
<td>ALPHA_ZZ</td>
<td>back stress - zz component</td>
</tr>
<tr>
<td>6</td>
<td>ALPHA_XY</td>
<td>back stress - xy component</td>
</tr>
<tr>
<td>7</td>
<td>ALPHA_YZ</td>
<td>back stress - yz component</td>
</tr>
<tr>
<td>8</td>
<td>ALPHA_ZX</td>
<td>back stress - zx component</td>
</tr>
<tr>
<td>9</td>
<td></td>
<td>tearing parameter</td>
</tr>
<tr>
<td>10</td>
<td></td>
<td>crack opening strain</td>
</tr>
<tr>
<td>11</td>
<td></td>
<td>crack opening direction - x component</td>
</tr>
<tr>
<td>12</td>
<td></td>
<td>crack opening direction - y component</td>
</tr>
<tr>
<td>13</td>
<td></td>
<td>crack opening direction - z component</td>
</tr>
<tr>
<td>14</td>
<td></td>
<td>flag for element death</td>
</tr>
</tbody>
</table>

### Table 8.30: State Variables for NEO HOOKEAN Model

This model has no state variables.

### Table 8.31: State Variables for ORTHOTROPIC CRUSH Model

<table>
<thead>
<tr>
<th>Name (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CRUSH</td>
<td>CRUSH</td>
<td></td>
</tr>
</tbody>
</table>

### Table 8.32: State Variables for ORTHOTROPIC RATE Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CRUSH</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 8.33: State Variables for PIEZO Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>STATE</td>
<td></td>
</tr>
</tbody>
</table>

Table 8.34: State Variables for POWER LAW CREEP Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ECREEP</td>
<td>equivalent creep strain</td>
</tr>
<tr>
<td>2</td>
<td>SEQDOT</td>
<td>equivalent stress rate</td>
</tr>
</tbody>
</table>

Table 8.35: State Variables for SHAPE MEMORY Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>STATE</td>
<td></td>
</tr>
</tbody>
</table>

Table 8.36: State Variables for SOIL FOAM Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>EVOL</td>
<td></td>
</tr>
</tbody>
</table>
### Table 8.37: State Variables for SWANSON Model

<table>
<thead>
<tr>
<th>Name (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SFJTH</td>
<td>SFJTH</td>
<td></td>
</tr>
<tr>
<td>RJTH</td>
<td>RJTH</td>
<td></td>
</tr>
<tr>
<td>V_MECH</td>
<td>VMECHXX</td>
<td></td>
</tr>
<tr>
<td></td>
<td>VMECHYY</td>
<td></td>
</tr>
<tr>
<td></td>
<td>VMECHZZ</td>
<td></td>
</tr>
<tr>
<td></td>
<td>VMECHXY</td>
<td></td>
</tr>
<tr>
<td></td>
<td>VMECHYZ</td>
<td></td>
</tr>
<tr>
<td></td>
<td>VMECHZX</td>
<td></td>
</tr>
<tr>
<td>SFJTH_FLAG</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Table 8.38: State Variables for THERMO EP POWER Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>EQPS</td>
<td>equivalent plastic strain</td>
</tr>
<tr>
<td>2</td>
<td>RADIUS</td>
<td>radius of yield surface</td>
</tr>
<tr>
<td>3</td>
<td>ALPHA_XX</td>
<td>back stress - xx component</td>
</tr>
<tr>
<td>4</td>
<td>ALPHA_YY</td>
<td>back stress - yy component</td>
</tr>
<tr>
<td>5</td>
<td>ALPHA_ZZ</td>
<td>back stress - zz component</td>
</tr>
<tr>
<td>6</td>
<td>ALPHA_XY</td>
<td>back stress - xy component</td>
</tr>
<tr>
<td>7</td>
<td>ALPHA_YZ</td>
<td>back stress - yz component</td>
</tr>
<tr>
<td>8</td>
<td>ALPHA_ZX</td>
<td>back stress - zx component</td>
</tr>
</tbody>
</table>
Table 8.39: State Variables for THERMO EP POWER WELD Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>EQPS</td>
<td></td>
<td>equivalent plastic strain</td>
</tr>
<tr>
<td>RADIUS</td>
<td></td>
<td>radius of yield surface</td>
</tr>
<tr>
<td>ALPHA_XX</td>
<td></td>
<td>back stress - xx component</td>
</tr>
<tr>
<td>ALPHA_YY</td>
<td></td>
<td>back stress - yy component</td>
</tr>
<tr>
<td>ALPHA_ZZ</td>
<td></td>
<td>back stress - zz component</td>
</tr>
<tr>
<td>ALPHA_XY</td>
<td></td>
<td>back stress - xy component</td>
</tr>
<tr>
<td>ALPHA_YZ</td>
<td></td>
<td>back stress - yz component</td>
</tr>
<tr>
<td>ALPHA_ZX</td>
<td></td>
<td>back stress - zx component</td>
</tr>
<tr>
<td>WELD_FLAG</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 8.40: State Variables for UNIVERSAL POLYMER Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AEND</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IGXX1 - IGXX20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IGYY1 - IGYY20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IGZZ1 - IGZZ20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IGXY1 - IGXY20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IGYZ1 - IGYZ20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IGZX1 - IGZX20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IKI11 - IKI120</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IKAT1 - IKAT20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IF1P1 - IF1P20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IF2J1 - IF2J20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>EPSXX</td>
<td></td>
<td></td>
</tr>
<tr>
<td>EPSYY</td>
<td></td>
<td></td>
</tr>
<tr>
<td>EPSZZ</td>
<td></td>
<td></td>
</tr>
<tr>
<td>EPSXY</td>
<td></td>
<td></td>
</tr>
<tr>
<td>EPSYZ</td>
<td></td>
<td></td>
</tr>
<tr>
<td>EPSZX</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LOGA</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 8.41: State Variables for VISCOELASTIC SWANSON Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SFJTH</td>
<td></td>
<td></td>
</tr>
<tr>
<td>JTH</td>
<td></td>
<td></td>
</tr>
<tr>
<td>VMECHXX</td>
<td></td>
<td></td>
</tr>
<tr>
<td>VMECHYY</td>
<td></td>
<td></td>
</tr>
<tr>
<td>VMECHZZ</td>
<td></td>
<td></td>
</tr>
<tr>
<td>VMECHXY</td>
<td></td>
<td></td>
</tr>
<tr>
<td>VMECHYZ</td>
<td></td>
<td></td>
</tr>
<tr>
<td>VMECHZX</td>
<td></td>
<td></td>
</tr>
<tr>
<td>VSXXDEV1 – VSXXDEV10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>VSYYDEV1 – VSYYDEV10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>VSZZDEV1 – VSZZDEV10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>VSXYDEV1 – VSXYDEV10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>VSYZDEV1 – VSYZDEV10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>VSZXDEV1 – VSZXDEV10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOXXDEV</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOYYDEV</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOZZDEV</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOXYDEV</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOYZDEV</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOZXDEV</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Table 8.42: State Variables for VISCOPLASTIC Model

<table>
<thead>
<tr>
<th>Index (Native Model)</th>
<th>Name (LAME Model)</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SVBXX</td>
<td></td>
</tr>
<tr>
<td></td>
<td>SVBYY</td>
<td></td>
</tr>
<tr>
<td></td>
<td>SVBZZ</td>
<td></td>
</tr>
<tr>
<td></td>
<td>SVBXY</td>
<td></td>
</tr>
<tr>
<td></td>
<td>SVBYZ</td>
<td></td>
</tr>
<tr>
<td></td>
<td>SVBZX</td>
<td></td>
</tr>
<tr>
<td></td>
<td>EQDOT</td>
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</tr>
<tr>
<td></td>
<td>COUNT</td>
<td></td>
</tr>
<tr>
<td></td>
<td>SHEAR</td>
<td></td>
</tr>
<tr>
<td></td>
<td>BULK</td>
<td></td>
</tr>
<tr>
<td></td>
<td>RATE</td>
<td></td>
</tr>
<tr>
<td></td>
<td>EXP</td>
<td></td>
</tr>
<tr>
<td></td>
<td>ALPHA</td>
<td></td>
</tr>
<tr>
<td></td>
<td>A1</td>
<td></td>
</tr>
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<td></td>
<td>A2</td>
<td></td>
</tr>
<tr>
<td></td>
<td>A4</td>
<td></td>
</tr>
<tr>
<td></td>
<td>A5</td>
<td></td>
</tr>
</tbody>
</table>
8.6. REGISTERED VARIABLES

8.6.2.5 Registered Variables for Shell/Membrane Material Models

Shell and membrane material models also make their state variables available through direct naming of the variables. Tables 8.43 through 8.46 indicate the names of the state variables for the shell material models.

Table 8.43: State Variables for Elastic-Plastic Model for Shells

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>eqps</td>
<td>Equivalent plastic strain</td>
</tr>
<tr>
<td>back_stress</td>
<td>Back stress</td>
</tr>
<tr>
<td>radius</td>
<td>Radius of the yield surface</td>
</tr>
</tbody>
</table>

Table 8.44: State Variables for Elastic-Plastic Power-Law Hardening Model for Shells

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>eqps</td>
<td>Equivalent plastic strain</td>
</tr>
<tr>
<td>radius</td>
<td>Radius of yield surface</td>
</tr>
</tbody>
</table>

Table 8.45: State Variables for Multilinear Elastic-Plastic Hardening Model for Shells

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>eqps</td>
<td>Equivalent plastic strain</td>
</tr>
<tr>
<td>tensile_eqps</td>
<td>Equivalent plastic strain only accumulated in tension</td>
</tr>
<tr>
<td>back_stress</td>
<td>Back stress</td>
</tr>
<tr>
<td>radius</td>
<td>Radius of the yield surface</td>
</tr>
</tbody>
</table>
Table 8.46: State Variables for Multilinear Elastic-Plastic Hardening Model with Failure for Shells

<table>
<thead>
<tr>
<th>Variable Name</th>
<th>Variable Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>eqps</td>
<td>Equivalent plastic strain</td>
</tr>
<tr>
<td>back_stress</td>
<td>Back stress</td>
</tr>
<tr>
<td>radius</td>
<td>Radius of the yield surface</td>
</tr>
<tr>
<td>tearing_parameter</td>
<td>The current value of the tearing parameter</td>
</tr>
<tr>
<td>crack_opening_strain</td>
<td>The value of the crack opening strain during the failure process</td>
</tr>
<tr>
<td>crack_flag</td>
<td>Status of the model: 0 for loading, 1 or 2 for initiation of failure, 3 during unloading</td>
</tr>
</tbody>
</table>
8.7 References


2. The eXtensible Data Model and Format (XDMF) . . . .

Chapter 9

User Subroutines

User-defines subroutines is a functionality shared by Adagio and Presto. This chapter discusses when and how to use user-defined subroutines. There are examples of user-defined subroutines in the latter part of this chapter. Some of the examples are code specific, i.e., they are applicable to Presto rather than Adagio or vice versa. All examples, regardless of their applicability, do provide important information about how to use the command options available for user-defined subroutines.

In the introductory part of Chapter 9, we first describe, in general, possible applications for the user subroutine functionality in Presto. Then, again in general, we describe the various pieces and steps that are required by the user to implement a user subroutine. Subsequently, we focus on various aspects of implementing the user subroutine functionality. Section 9.1 describes the details of the user subroutine. Section 9.2 describes the command lines associated with user subroutines that appear in the Presto input file. In Section 9.3, we explain how to build and use a version of Presto that incorporates your user subroutine. Finally, Section 9.4 provides examples of actual user subroutines, and Section 9.5 lists some subroutines that are now in the standard user library.

Applications. User subroutines are primarily intended as complex function evaluators that are to be used in conjunction with existing Presto capability (boundary conditions, element death, user output, etc.). For example, suppose we want to have a prescribed displacement boundary condition applied to a set of nodes, and we want the displacement at each node to vary with both time and spatial location of the node. The standard function option associated with the prescribed direction displacement boundary condition in Presto only allows for time variation; i.e., at any given time, the direction and the magnitude of the displacement at each node, regardless of the spatial location of the node, are the same. If we wanted to have a spatial variation of the displacement field in addition to the time variation, it would be necessary to implement a user subroutine for the prescribed direction displacement boundary condition. Other examples of possible uses of user subroutines are as follows:

- Element death is determined by a complex function based on a set of physical parameters and element stress.
- The user wants to compute the total contact force acting on a given surface.
• Element stress information must be transformed to a local coordinate system so that the stress values will be meaningful.

• An aerodynamic pressure based on velocity and surface normal is applied to a specified surface.

Some capability exists for using mesh connectivity. It is possible to compute an element quantity based on values at the element nodes.

Some difficulties might occur in parallel applications. If computations for element A depend on quantities in element B and elements A and B are on different processors, then the computations for A may not have access to quantities in element B. For most computations in user subroutines, however, this should not be a problem.

Implementing completely new capabilities, particularly if these capabilities involve parallel computing, may be difficult or impossible with user subroutines.

**General Pieces and Steps.** A number of pieces and steps are required to make use of user subroutines. Here, we present a brief description of the pieces and steps that a user will need for user subroutines without going into detail. The details are discussed in later parts of this chapter.

1. You must first determine whether your application fits in the user subroutine format. This can be done by considering the above requirements and examining the description of commands for functionality in Presto. For example, the basic kinematic boundary conditions and force conditions allow for the use of user subroutines. The description of these commands includes a discussion of how a user subroutine could be applied and what command line will invoke a user subroutine.

2. If you determine that your application can make use of the user subroutine functionality in Presto, you will then need to write the subroutine. The parts of the subroutine that interface to Presto have specified formats. The details of these interfaces are described in later sections. One part of the subroutine with a specified format is the call list. Other parts of the subroutine with a specified format are code that will do the following:

   - Read parameters from the Presto input file
   - Access a variety of information—field variables, analysis time, etc.—from Presto
   - Store computed quantities

Parameters are values they may be passed from the Presto input file to the user subroutine. Suppose that the spatial variation for some quantity in the user subroutine uses some characteristic length and the user wishes to examine results generated by using several different values of the characteristic length. By setting up the characteristic length as a parameter, the value for the parameter in the user subroutine can easily be changed by changing the value for the parameter in the input file. This lets the user change the value for a variable inside the user subroutine without having to recompile the user subroutine.
The portion of your subroutine not built on the Presto specifications will reflect your specific application. The code to implement your application may include a loop over nodes that prescribes a displacement based on the current time for the analysis and the spatial location of the node.

3. After you write the user subroutine, you will need to have a command line in your input file that tells Presto you want to use the user subroutine you have written. For example, if your user subroutine is a specialized prescribed displacement boundary condition, then inside a PRESCRIBED DISPLACEMENT command block, you will have a command line of the form

   NODE_SET_SUBROUTINE = <string>subroutine_name

that provides the name of your user subroutine.

4. Following the invocation of the user subroutine, there may be command lines for various parameters associated with the user subroutine. There may also be some additional command lines in other sections of the code required for your application. For example, you may have to add command lines in the region scope that will create an internal variable associated with a computed quantity so that the computed quantity can be written to the results file.

5. Once you have constructed the user subroutine, which is a FORTRAN file, and the Presto input file, you can build an executable version of Presto that will run your user subroutine. Your Presto run will then incorporate the functionality you have created in your user subroutine.

Figure 9.1 presents a very high-level overview of the various components that work together to implement the user subroutine functionality. The two main components needed for user subroutines, which are commands in the Presto input file and the actual user subroutine, are represented by the two columns in Figure 9.1.
Figure 9.1: Overview of components required to implement user subroutine functionality, excluding compilation and execution commands.
9.1 User Subroutines: Programming

Currently, user subroutines are only supported in FORTRAN 77. Any subroutine that can be compiled with a FORTRAN 77 compiler on the target execution machine can be used. The user should be aware that some computers support different FORTRAN language extensions than others. (In the future, other languages such as FORTRAN 90, C, and C++ may be supported.)

User subroutine variable types must interface directly with the matching variable types used in the main Presto code. Thus, the FORTRAN 77 subroutines should use only integer, double precision, or character types for any data used in the interface or in any query function. Using the wrong data type may yield unpredictable results. The methods used to pass character types from Presto to FORTRAN user subroutines can be machine-dependent, but generally this functionality works quite well.

The basic structure for the user subroutine is as follows:

```
subroutine sub_name(call list)
    {declaration of variables}
    {retrieve parameters from Presto input file}
    {query Presto for information}
    {application-specific code
        ...
    }
    {write computed values}
END
```

In general, the user will begin the subroutine with variable declarations. After the variable declarations, the user can then query the Presto input file for parameters. Additional Presto information such as field variables or element topology can then be retrieved from Presto. Once the user has collected all the information for the application, the application-specific portion of the code can be written. After the application-specific code is complete, the user may store computed values.

Section 9.1.1 through Section 9.1.3 describe in detail the format for the interfaces to Presto that will allow the user to make the subroutine call, retrieve information from Presto, and write computed values. In these sections, mesh entities can be a node, an element face, or an element.
9.1.1 Subroutine Interface

The following interface is used for all user subroutines:

```
subroutine sub_name(int num_objects,
                 int num_values,
                 real evaluation_time,
                 int object_ids[],
                 real output_values[],
                 int output_flags[],
                 int error_code)
```

The name of the user subroutine, `sub_name`, is selected by the user. Avoid names for the subroutine that are longer than 10 characters. This may cause build problems on some systems.

A detailed description of the input and output parameters is provided in Table 9.1 and Table 9.2.

<table>
<thead>
<tr>
<th>Input Parameter</th>
<th>Data Type</th>
<th>Parameter Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_objects</td>
<td>Integer</td>
<td>Number of input mesh entities. For example, if the subroutine is a node set subroutine, this would be the number of nodes on which the subroutine will operate.</td>
</tr>
<tr>
<td>num_values</td>
<td>Integer</td>
<td>Number of return values. This is the number of values per mesh entity.</td>
</tr>
<tr>
<td>evaluation_time</td>
<td>Real</td>
<td>Time at which the subroutine should be evaluated. This may vary slightly from the current analysis time. Velocities for example are evaluated one-half time step ahead.</td>
</tr>
<tr>
<td>object_ids</td>
<td>Integer</td>
<td>Array of mesh-entity identification numbers. The array has a length of num_objects. The input numbers are the global numbers of the input objects. The object identification numbers can be used to query information about a mesh entity.</td>
</tr>
</tbody>
</table>

9.1.2 Query Functions

Presto follows a design philosophy for user subroutines that a minimal amount of information should be passed through the call list. Additional information may be queried from within the subroutine. A user subroutine may query a wide variety of information from Presto.
Table 9.2: Subroutine Output Parameters

<table>
<thead>
<tr>
<th>Output Parameter</th>
<th>Data Type</th>
<th>Parameter Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>output_values (num_values, num_objects)</td>
<td>Integer</td>
<td>Array of output values computed by the subroutine. The number of output values will be either the number of mesh entities or some multiple of the number of mesh entities. For example, if there were six nodes (num_objects equals 6) and one value was to be computed per node, the length of output_values would be 6. Similarly, if there were six nodes (num_objects equals 6) and three values were to be computed for each node (as for acceleration, which has X-, Y-, and Z-components), the length of output_values would be 18.</td>
</tr>
<tr>
<td>output_flags (num_objects)</td>
<td>Integer</td>
<td>Array of returned flags for each set of data values. When used, this array will generally have a length of num_objects. The usage of the flags depends on subroutine type; the flags are currently used only for element death and for kinematic boundary conditions. For the kinematic boundary conditions (displacement, velocity, acceleration) a flag of –1 means ignore the constraint, a flag of 0 means set the absolute constraint value, and a flag of 1 means set the constraint with direction and distance.</td>
</tr>
<tr>
<td>error_code</td>
<td>Integer</td>
<td>Error code returned by the user subroutine. A value of 0 indicates no errors. Any value other than zero is an error. If the return value is nonzero, Presto will report the error code and terminate the analysis.</td>
</tr>
</tbody>
</table>
9.1.2.1 Parameter Query

A number of user subroutine parameters may be set as described in Section 9.2.2.3. These subroutine parameters can be obtained from the Presto input file via the query functions listed below.

\begin{verbatim}
  aupst_get_real_param(string var_name, real var_value, int error_code)
  aupst_get_integer_param(string var_name, int var_value, int error_code)
  aupst_get_string_param(string var_name, string var_value, int error_code)
\end{verbatim}

All three of these subroutine calls are tied to a corresponding “parameter” command line that will appear in the Presto input file. The parameter command lines are described in Section 9.2.2.3. These command lines are named based on the type of value they store, i.e., SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER.

We will use the example of a real parameter to show how the subroutine call works in conjunction with the SUBROUTINE REAL PARAMETER command line. Suppose we have a real parameter radius that is set to a value of 2.75 on the SUBROUTINE REAL PARAMETER command line:

\begin{verbatim}
SUBROUTINE REAL PARAMETER: radius = 2.75
\end{verbatim}

Also suppose we have a call to aupst_get_real_parameter in the user subroutine:

\begin{verbatim}
call aupst_get_real_parameter("radius", cyl_radius, error_code)
\end{verbatim}

In the call to aupst_get_real_parameter, we have \texttt{var_name} set to \texttt{radius} and \texttt{var_value} defined as the real FORTRAN variable \texttt{cyl_radius}. The call to aupst_get_real_parameter will assign the value 2.75 to the FORTRAN variable \texttt{cyl_radius}. A similar pattern is followed for integer and string parameters.

The arguments for the parameter-related query functions are described in Table 9.3, Table 9.4, and Table 9.5. The function is repeated prior to each table for easy reference.
### Table 9.3: aupst_get_real_param Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>var_name</td>
<td>Input</td>
<td>String</td>
<td>Name of a real-valued subroutine parameter, as defined in the Presto input file via the <code>SUBROUTINE REAL PARAMETER</code> command line.</td>
</tr>
<tr>
<td>var_value</td>
<td>Output</td>
<td>Real</td>
<td>Name of a real variable to be used in the FORTRAN subroutine. The FORTRAN variable var_value will be set to the value specified by the <code>SUBROUTINE REAL PARAMETER</code> command line.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the parameter value from the input file. If the retrieval is successful, error_code is set to 0. If the parameter is not found or is the wrong type, error_code is set to a value other than 0.</td>
</tr>
</tbody>
</table>
aupst_get_integer_param(string var_name, int var_value, int error_code)

Table 9.4: aupst_get_integer_param Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>var_name</td>
<td>Input</td>
<td>String</td>
<td>Name of an integer-valued subroutine parameter, as defined in the Presto input file via the <code>SUBROUTINE INTEGER PARAMETER</code> command line.</td>
</tr>
<tr>
<td>var_value</td>
<td>Output</td>
<td>Integer</td>
<td>Name of an integer variable to be used in the FORTRAN subroutine. The FORTRAN variable var_value will be set to the value specified by the <code>SUBROUTINE INTEGER PARAMETER</code> command line.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the parameter value from the input file. If the retrieval is successful, error_code is set to 0. If the parameter is not found or is the wrong type, error_code is set to a value other than 0.</td>
</tr>
</tbody>
</table>
aupst_get_string_param(string var_name, string var_value, int error_code)

Table 9.5: aupst_get_string_param Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>var_name</td>
<td>Input</td>
<td>String</td>
<td>Name of a string-valued subroutine parameter, as defined in the Presto input file via the SUBROUTINE STRING PARAMETER command line.</td>
</tr>
<tr>
<td>var_value</td>
<td>Output</td>
<td>String</td>
<td>Name of a string variable to be used in the FORTRAN subroutine. The FORTRAN variable var_value will be set to the value specified by the SUBROUTINE STRING PARAMETER command line.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the parameter value from the input file. If the retrieval is successful, error_code is set to 0. If the parameter is not found or is the wrong type, error_code is set to a value other than 0.</td>
</tr>
</tbody>
</table>
9.1.2.2 Function Data Query

The function data query routine listed below may be used for extracting data from a function that is defined in a `DEFINITION FOR FUNCTION` command block in the Presto input file. This query allows the user to directly access information stored in a function defined in the Presto input file.

```
aupst.evaluate_function(string func_name, real input_times[], int num_times, real output_data[])
```

The arguments for this function are described in Table 9.6.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>func_name</code></td>
<td>Input</td>
<td>String</td>
<td>Name of the function to look up.</td>
</tr>
<tr>
<td><code>input_times</code></td>
<td>Input</td>
<td>Real</td>
<td>Array of times used to extract values of the function.</td>
</tr>
<tr>
<td><code>num_times</code></td>
<td>Input</td>
<td>Integer</td>
<td>Length of the array <code>input_times</code>.</td>
</tr>
<tr>
<td><code>output_data</code></td>
<td>Output</td>
<td>Real</td>
<td>Array of output values of the named function at the specified times.</td>
</tr>
</tbody>
</table>

9.1.2.3 Time Query

The time query function can be used to determine the current analysis time. This is the time associated with the new time step. This time may not be equivalent to the `evaluation_time` argument passed into the subroutine (see Section 9.1.1, Table 9.1) as some boundary conditions need to be evaluated at different times than others. The parameter of the time query function listed below is given in Table 9.7.

```
aupst.get_time(real time)
```

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>time</code></td>
<td>Output</td>
<td>Real</td>
<td>Current analysis time.</td>
</tr>
</tbody>
</table>

9.1.2.4 Field Variables

Field variables (displacements, stresses, etc.) may be defined on groups of mesh entities. A number of queries are available for getting and putting field variables. These queries involve passing in a set of mesh-entity identification numbers to receive field values on the mesh entities. There are
query functions to check for the existence and size of a field, functions to retrieve the field values, and functions to store new variables in a field. The field query functions listed below can be used to extract any registered nodal or element variable field.

```c
aupst_check_node_var(int num_nodes, int num_components,
                      int node_ids[], string var_name,
                      int error_code)

aupst_check_elem_var(int num_elems, int num_components,
                      int elem_ids[], string var_name,
                      int error_code)

aupst_get_node_var(int num_nodes, int num_components,
                    int node_ids[], real return_data[],
                    string var_name, int error_code)

aupst_get_elem_var(int num_elems, int num_components,
                    int elem_ids[], real return_data[],
                    string var_name, int error_code)

aupst_put_node_var(int num_nodes, int num_components,
                    int node_ids[], real new_data[],
                    string var_name, int error_code)

aupst_put_elem_var(int num_elems, int num_components,
                    int elem_ids[], real new_data[],
                    string var_name, int error_code)
```

The arrays where data are stored are static arrays. These arrays of a set size will be declared at the beginning of a user subroutine. The query functions to check for the existence and size of a field can be used to ensure that the size of the array of information being returned from Presto does not exceed the size of the array allocated by the user.

The arguments to field query functions are defined in Table 9.8 through Table 9.13. The function is repeated before each table for easy reference.
aupst_check_node_var(int num_nodes, int num_components,
    int node_ids[], string var_name,
    int error_code)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_nodes</td>
<td>Input</td>
<td>Integer</td>
<td>Number of nodes used to extract field information.</td>
</tr>
<tr>
<td>num_components</td>
<td>Output</td>
<td>Integer</td>
<td>Number of components in the field information. A displacement field at a node has three components, for example.</td>
</tr>
<tr>
<td>node_ids (num_nodes)</td>
<td>Input</td>
<td>Integer</td>
<td>Array of size num_nodes listing the node identification number for each node where field information will be retrieved.</td>
</tr>
<tr>
<td>var_name</td>
<td>Input</td>
<td>String</td>
<td>Name of the field variable. The field variable must be a registered Presto variable.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the field. If the retrieval is successful, error_code is set to 0. If a nonzero value is returned for error_code, the field variable does not exist or is not defined on one or more of the input nodes.</td>
</tr>
</tbody>
</table>
aupst_check_elem_var(int num_elems, int num_components,
        int elem_ids[], string var_name,
        int error_code)

Table 9.9: aupst_check_elem_var Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_elems</td>
<td>Input</td>
<td>Integer</td>
<td>Number of elements used to extract field information.</td>
</tr>
<tr>
<td>num_components</td>
<td>Output</td>
<td>Integer</td>
<td>Number of components in the field information. A stress field for an eight-node hexahedron element has six components, for example.</td>
</tr>
<tr>
<td>elem_ids</td>
<td>Input</td>
<td>Integer</td>
<td>Array of size num_elems listing the element identification number for each element where field information will be retrieved.</td>
</tr>
<tr>
<td>var_name</td>
<td>Input</td>
<td>String</td>
<td>Name of the field variable. The field variable must be a registered Presto variable.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the field. If the retrieval is successful, error_code is set to 0. If a nonzero value is returned for error_code, the field variable does not exist or is not defined on one or more of the input nodes.</td>
</tr>
</tbody>
</table>
aupst_get_node_var(int num_nodes, int num_components,
               int node_ids[], real return_data[],
               string var_name, int error_code)

Table 9.10: aupst_get_node_var Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_nodes</td>
<td>Input</td>
<td>Integer</td>
<td>Number of nodes used to extract field information.</td>
</tr>
<tr>
<td>num_components</td>
<td>Input</td>
<td>Integer</td>
<td>Number of components in the field information. A displacement field at a</td>
</tr>
<tr>
<td>node_ids</td>
<td>Input</td>
<td>Integer</td>
<td>node has three components, for example.</td>
</tr>
<tr>
<td>(num_nodes)</td>
<td></td>
<td></td>
<td>Array of size num_nodes listing the node identification number for each node</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>where field information will be retrieved.</td>
</tr>
<tr>
<td>return_data</td>
<td>Output</td>
<td>Real</td>
<td>Array of size num_components $\times$ num_nodes containing the field data at</td>
</tr>
<tr>
<td>(num_components, num_nodes)</td>
<td></td>
<td></td>
<td>each node.</td>
</tr>
<tr>
<td>var_name</td>
<td>Input</td>
<td>String</td>
<td>Name of the field variable. The field variable must be a registered Presto</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>variable.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the field. If the retrieval is</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>successful, error_code is set to 0. If a nonzero value is returned for</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>error_code, the field variable does not exist or is not defined on one or</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>more of the input nodes.</td>
</tr>
</tbody>
</table>
aupst_get_elem_var(int num_elems, int num_components,
       int elem_ids[], real return_data[],
       string var_name, int error_code)

Table 9.11: aupst_get_elem_var Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_elems</td>
<td>Input</td>
<td>Integer</td>
<td>Number of elements used to extract field information.</td>
</tr>
<tr>
<td>num_components</td>
<td>Input</td>
<td>Integer</td>
<td>Number of components in the field information. A stress field for a an eight-node hexahedron element has six components, for example.</td>
</tr>
<tr>
<td>elem_ids</td>
<td>Input</td>
<td>Integer</td>
<td>Array of size num_elems listing the element identification number for each element where field information will be retrieved.</td>
</tr>
<tr>
<td>return_data</td>
<td>Output</td>
<td>Real</td>
<td>Array of size num_components × num_elems containing the field data for each element.</td>
</tr>
<tr>
<td>var_name</td>
<td>Input</td>
<td>String</td>
<td>Name of the field variable. The field variable must be a registered Presto variable.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the field. If the retrieval is successful, error_code is set to 0. If a nonzero value is returned for error_code, the field variable does not exist or is not defined on one or more of the input nodes.</td>
</tr>
</tbody>
</table>
**aupst_put_node_var**(int num_nodes, int num_components, int node_ids[], real new_data[], string var_name, int error_code)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_nodes</td>
<td>Input</td>
<td>Integer</td>
<td>Number of nodes for which the user will specify the field data.</td>
</tr>
<tr>
<td>num_components</td>
<td>Input</td>
<td>Integer</td>
<td>Number of components in the field information. A displacement field at a node has three components, for example.</td>
</tr>
<tr>
<td>node_ids</td>
<td>Input</td>
<td>Integer</td>
<td>Array of size num_nodes listing the node identification number for each node where field information will be retrieved.</td>
</tr>
<tr>
<td>(num_nodes)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>new_data</td>
<td>Input</td>
<td>Real</td>
<td>Array of size num_components × num_nodes containing the new data for the field.</td>
</tr>
<tr>
<td>(num_components, num_nodes)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>var_name</td>
<td>Input</td>
<td>String</td>
<td>Name of the field variable. The field variable must be a registered Presto variable.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the field. If the retrieval is successful, error_code is set to 0. If a nonzero value is returned for error_code, the field variable does not exist or is not defined on one or more of the input nodes.</td>
</tr>
</tbody>
</table>

Table 9.12: aupst_put_node_var Arguments
9.1. USER SUBROUTINES: PROGRAMMING

aupst_put_elem_var(int num elems, int num_components,
                   int elem_ids[], real new_data[],
                   string var_name, int error_code)

Table 9.13: aupst_put_elem_var Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num elems</td>
<td>Input</td>
<td>Integer</td>
<td>Number of elements for which the user will specify the field data.</td>
</tr>
<tr>
<td>num_components</td>
<td>Input</td>
<td>Integer</td>
<td>Number of components in the field information. A stress field for an eight-node hexahedron element has six components, for example.</td>
</tr>
<tr>
<td>elem_ids</td>
<td>Input</td>
<td>Integer</td>
<td>Array of size num elems listing the element identification number for each element where field information will be retrieved.</td>
</tr>
<tr>
<td>new_data</td>
<td>Input</td>
<td>Real</td>
<td>Array of size num_components × num_elems containing the new data for the field.</td>
</tr>
<tr>
<td>var_name</td>
<td>Input</td>
<td>String</td>
<td>Name of the field variable. The field variable must be a registered Presto variable.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the field. If the retrieval is successful, error_code is set to 0. If a nonzero value is returned for error_code, the field variable does not exist or is not defined on one or more of the input nodes.</td>
</tr>
</tbody>
</table>

9.1.2.5 Global Variables

Global variables may be extracted or set from user subroutines. A global variable has a single value for a given region.

Global variables have limited support for parallel operations. There are two subroutines to perform parallel modification of global variables: **aupst_put_global_var** and **aupst_local_put_global_var**.

- The subroutine **aupst_local_put_global_var** only modifies a temporary local copy of the global variable. The local copies on the various processors are reduced to create the
true global value at the end of the time step. Global variables set with `aupst_local_put_global_var` do not have the single processor value available immediately. The true global variable will not be available through the `aupst_get_global_var` routine until the next time step.

- The subroutine `aupst_put_global_var` attempts to immediately modify and perform a parallel reduction of the value of a global variable. Care must be taken to call this routine on all processors at the same time with the same arguments. Failure to call the routine from all processors will result in the code hanging. For some types of subroutines this is not possible or reliable. For example, a boundary condition subroutine may not be called at all on a processor that contains no nodes in the set of nodes assigned to the boundary condition. It is recommended that `aupst_local_put_global_var` only be used in conjunction with a user subroutine referenced in a USER OUTPUT command block (Section 8.1.2).

Only user-defined global variables may be modified by the user subroutine (see Section 9.2.4). However, any global variable that exists on the region may be checked or extracted. The following subroutine calls pertain to global variables:

```
aupst_get_global_var(int num_comp, real return_data,
                      string var_name, int error_code)

aupst_put_global_var(int num_comp, real input_data,
                      string reduction_type,
                      string var_name, int error_code)

aupst_local_put_global_var(int num_comp, real input_data,
                           string var_name, string reduction_type,
                           int error_code)
```

The arguments for subroutine calls pertaining to global variables are defined in Table 9.14 through Table 9.17. The call is repeated before each table for easy reference.
9.1. USER SUBROUTINES: PROGRAMMING

```c
aupst_check_global_var(int num_comp, string var_name
    int error_code)
```

Table 9.14: `aupst_check_global_var` Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_comp</td>
<td>Output</td>
<td>Integer</td>
<td>Number of components of the global variable.</td>
</tr>
<tr>
<td>var_name</td>
<td>Input</td>
<td>String</td>
<td>Name of the global variable.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of accessing the global variable.</td>
</tr>
</tbody>
</table>

A nonzero value of `error_code` means the global variable does not exist or in some way cannot be accessed.

```c
aupst_get_global_var(int num_comp, real return_data,
    string var_name, int error_code)
```

Table 9.15: `aupst_get_global_var` Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_comp</td>
<td>Input</td>
<td>Integer</td>
<td>Number of components of the global variable.</td>
</tr>
<tr>
<td>return_data</td>
<td>Output</td>
<td>Real</td>
<td>Value of the global variable.</td>
</tr>
<tr>
<td>var_name</td>
<td>Input</td>
<td>String</td>
<td>Name of the global variable.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of accessing the global variable.</td>
</tr>
</tbody>
</table>

A nonzero value of `error_code` means the global variable does not exist or in some way cannot be accessed.
aupst_put_global_var(int num_comp, real input_data,
               string reduction_type,
               string var_name, int error_code)

Table 9.16: aupst_put_global_var Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_comp</td>
<td>Input</td>
<td>Integer</td>
<td>Number of components of the global variable.</td>
</tr>
<tr>
<td>input_data</td>
<td>Input</td>
<td>Real</td>
<td>New value of the global variable.</td>
</tr>
<tr>
<td>reduction_type</td>
<td>Input</td>
<td>String</td>
<td>Type of parallel reduction to perform on the variable. Options are “sum”,</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>“min”, “max”, and “none”.</td>
</tr>
<tr>
<td>var_name</td>
<td>Input</td>
<td>String</td>
<td>Name of the global variable.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of accessing the global variable. If there is</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>no error in accessing this variable, error_code is set to 0. A nonzero</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>value of error_code means the global variable does not exist, in some way</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>cannot be accessed, or may not be overwritten.</td>
</tr>
</tbody>
</table>
```c
aupst_local_put_global_var(int num_comp, real input_data,
                        string var_name,
                        string reduction_type,
                        int error_code)
```

**Table 9.17: aupst_local_put_global_var Arguments**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_comp</td>
<td>Input</td>
<td>Integer</td>
<td>Number of components of the global variable.</td>
</tr>
<tr>
<td>input_data</td>
<td>Input</td>
<td>Real</td>
<td>New value of the global variable.</td>
</tr>
<tr>
<td>reduction_type</td>
<td>Input</td>
<td>String</td>
<td>Type of parallel reduction to perform on the variable. Options are “sum”, “min”, and “max”. The operation type specified here must match the operation type given to the user-defined global variable when it is defined in the Presto input file.</td>
</tr>
<tr>
<td>var_name</td>
<td>Input</td>
<td>String</td>
<td>Name of the global variable.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of accessing the global variable. If there is no error in accessing this variable, error_code is set to 0. A nonzero value of error_code means the global variable does not exist, in some way cannot be accessed, or may not be overwritten.</td>
</tr>
</tbody>
</table>

### 9.1.2.6 Topology Extraction

The element and surface subroutines operate on groups of elements or faces. The elements and faces may have a variety of topologies. Topology queries can be used to get topological data about elements and faces. The topology of an object is represented by an integer. The integer is formed from a function of the number of dimensions, vertices, and nodes of an object. The topology of an object is given by:

\[
topology = \text{num_node} + 100 \times \text{num_vert} + 10000 \times \text{num_dim}
\]

In a FORTRAN routine, the number of nodes can easily be extracted with the mod function:

```fortran
num_node = mod(topo,100)
num_vert = mod(topo / 100, 100)
num_dim = mod(topo / 10000, 100)
```
Table 9.18: Topologies Used by Presto

<table>
<thead>
<tr>
<th>Topology</th>
<th>Element / Face Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>00101</td>
<td>One-node particle</td>
</tr>
<tr>
<td>10202</td>
<td>Two-node beam, truss, or damper</td>
</tr>
<tr>
<td>20404</td>
<td>Four-node quadrilateral</td>
</tr>
<tr>
<td>20303</td>
<td>Three-node triangle</td>
</tr>
<tr>
<td>20304</td>
<td>Four-node triangle</td>
</tr>
<tr>
<td>20306</td>
<td>Six-node triangle</td>
</tr>
<tr>
<td>30404</td>
<td>Four-node tetrahedron</td>
</tr>
<tr>
<td>30408</td>
<td>Eight-node tetrahedron</td>
</tr>
<tr>
<td>30410</td>
<td>Ten-node tetrahedron</td>
</tr>
<tr>
<td>30808</td>
<td>Eight-node hexahedron</td>
</tr>
</tbody>
</table>

Table 9.18 lists the topologies currently in use by Presto.

The following topology query functions are available in Presto:

```
aupst_get_elem_topology(int num elems, int elem_ids[],
                        int topology[], int error_code)
```

```
aupst_get_elem_nodes(int num elems, int elem_ids[],
                      int elem_node_ids[], int error_code)
```

```
aupst_get_face_topology(int num faces, int face_ids[],
                         int topology[], int error_code)
```

```
aupst_get_face_nodes(int num faces, int face_ids[],
                      int face_node_ids[], int error_code)
```

The arguments for the topology extraction functions are defined in Table 9.19 through Table 9.22. The function is repeated before each table for easy reference.
aupst_get_elem_topology(int num elems, int elem_ids[], int topology[], int error_code)

Table 9.19: aupst_get_elem_topology Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num elems</td>
<td>Input</td>
<td>Integer</td>
<td>Number of elements from which the topology will be extracted.</td>
</tr>
<tr>
<td>elem_ids (num elems)</td>
<td>Input</td>
<td>Integer</td>
<td>Array of length num elems listing the element identification for each element from which the topology will be extracted.</td>
</tr>
<tr>
<td>topology (num elems)</td>
<td>Output</td>
<td>Integer</td>
<td>Array of length num elems that has the topology for each element. See Table 8.18.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the element identification numbers. If the retrieval is successful, error_code is set to 0. A nonzero value is returned for error_code if one of the element identification numbers is not valid.</td>
</tr>
</tbody>
</table>
The function `aupst_get_elem_nodes` is defined as:

```c
aupst_get_elem_nodes(int num_elems, int elem_ids[],
                     int elem_node_ids[], int error_code)
```

## Table 9.20: `aupst_get_elem_nodes` Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>num_elems</code></td>
<td>Input</td>
<td>Integer</td>
<td>Number of elements from which the topology will be extracted.</td>
</tr>
<tr>
<td><code>elem_ids</code> (num elems)</td>
<td>Input</td>
<td>Integer</td>
<td>Array of length num_elems listing the element identification for each element from which the topology will be extracted.</td>
</tr>
<tr>
<td><code>elem_node_ids</code> (number of nodes for element type × num_elems)</td>
<td>Output</td>
<td>Integer</td>
<td>Array containing the node identification numbers for each element requested. The length of the array is the total number of nodes contained in all elements. If the elements are eight-node hexahedra, then the number of nodes will be 8 × num_elems. The first set of eight entries in the array will be the eight nodes defining the first element. The second set of eight entries will be the eight nodes defining the second element, and so on.</td>
</tr>
<tr>
<td><code>error_code</code></td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the element identification numbers. If the retrieval is successful, error_code is set to 0. A nonzero value is returned for error_code if one of the element identification numbers is not valid.</td>
</tr>
</tbody>
</table>
9.1. USER SUBROUTINES: PROGRAMMING

```
aupst_get_face_topology(int num_faces, int face_ids[],
                        int topology[], int error_code)
```

Table 9.21: aupst_get_face_topology Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num_faces</td>
<td>Input</td>
<td>Integer</td>
<td>Number of faces from which the topology will be extracted.</td>
</tr>
<tr>
<td>face_ids</td>
<td>Input</td>
<td>Integer</td>
<td>Array of length num_faces listing the face identification for each face from which the topology will be extracted.</td>
</tr>
<tr>
<td>topology</td>
<td>Output</td>
<td>Integer</td>
<td>Array of length num_faces containing the output topologies of each face.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the face identification numbers. If the retrieval is successful, error_code is set to 0. A nonzero value is returned for error_code if one of the face identification numbers is not valid.</td>
</tr>
</tbody>
</table>
```c
aupst_get_face_nodes(int num_faces, int face_ids[],
                   int face_node_ids[], int error_code)
```

Table 9.22: `aupst_get_face_nodes` Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>num_faces</code></td>
<td>Input</td>
<td>Integer</td>
<td>Number of faces from which the topology will be extracted.</td>
</tr>
<tr>
<td><code>face_ids</code></td>
<td>Input</td>
<td>Integer</td>
<td>Array of length <code>num_faces</code> listing the face identification for each face from which the topology will be extracted.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><code>face_node_ids</code></td>
<td>Output</td>
<td>Integer</td>
<td>Array containing the node identification numbers for each face requested. The length of the array is the total number of nodes contained in all faces. If the faces are four-node quadrilaterals, then the number of nodes will be <code>4 × num_faces</code>. The first set of four entries in the array will be the four nodes defining the first face. The second set of four entries will be the four nodes defining the second face, and so on.</td>
</tr>
<tr>
<td><code>error_code</code></td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the face identification numbers. If the retrieval is successful, <code>error_code</code> is set to 0. A nonzero value is returned for <code>error_code</code> if one of the face identification numbers is not valid.</td>
</tr>
</tbody>
</table>
9.1.3 Miscellaneous Query Functions

A number of miscellaneous query functions are available for computing some commonly used quantities.

```
aupst_get_one_elem_centroid(int num_elems, int elem_ids[],
real centroids, int error_code)
aupst_get_point(string point_name, real point_coords,
int error_code)
aupst_get_proc_num(proc_num)
```

The arguments for the miscellaneous query functions are defined in Table 9.23 through Table 9.25. The function is repeated before each table for easy reference.

```
aupst_get_one_elem_centroid(int num_elems, int elem_ids[],
real centroids[], int error_code)
```

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>num elems</td>
<td>Input</td>
<td>Integer</td>
<td>Number of elements for which to extract the topology.</td>
</tr>
<tr>
<td>elem_ids</td>
<td>Input</td>
<td>Integer</td>
<td>Array of length num_elems listing the element identification for each element for which the centroid will be computed.</td>
</tr>
<tr>
<td>(num elems)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>centroids</td>
<td>Output</td>
<td>Real</td>
<td>Array of length 3 × num_elems containing the centroid of each element.</td>
</tr>
<tr>
<td>(3, num elems)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the element identification numbers. If the retrieval is successful, error_code is set to 0. A nonzero value is returned for error_code if one of the element identification numbers is not valid.</td>
</tr>
</tbody>
</table>
aupst_get_point(string point_name, real point_coords, int error_code)

Table 9.24: aupst_get_point Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>point_name</td>
<td>Input</td>
<td>String</td>
<td>SIERRA name for a given point.</td>
</tr>
<tr>
<td>point_coords</td>
<td>Output</td>
<td>Real</td>
<td>Array of length 3 containing the x, y, and z coordinates of the point.</td>
</tr>
<tr>
<td>error_code</td>
<td>Output</td>
<td>Integer</td>
<td>Error code indicating status of retrieving the point. If the retrieval is successful, error_code is set to 0. A nonzero value is returned for error_code if the point cannot be found</td>
</tr>
</tbody>
</table>

aupst_get_proc_num(proc_num)

Table 9.25: aupst_get_proc_num Arguments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Usage</th>
<th>Data Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>proc_num</td>
<td>Output</td>
<td>Integer</td>
<td>Processor number of the calling process. This number can be used for informational purposes. A common example is that output could only be written by a single processor, e.g., processor 0, rather than by all processors.</td>
</tr>
</tbody>
</table>
9.2 User Subroutines: Command File

In addition to the actual user subroutine, you will need to add command lines to your input file to make use of your user subroutine. This section describes the command lines that are used in conjunction with user subroutines. This section also describes two additional command blocks, TIME STEP INITIALIZATION and USER VARIABLE. The TIME STEP INITIALIZATION command block lets you execute a user subroutine at the beginning of a time step as opposed to some later time. The USER VARIABLE command block can be used in conjunction with user subroutines or for user-defined output.

9.2.1 Subroutine Identification

As described in Section 2.1.4, there is one command line associated with the user subroutine functionality that must be provided in the domain scope:

```plaintext
USER SUBROUTINE FILE = <string>file_name
```

The named file may contain one or more user subroutines. The file must have an extension of “.F”, as in blast.F.

9.2.2 User Subroutine Command Lines

```plaintext
{begin command block}
NODE SET SUBROUTINE = <string>subroutine name | 
SURFACE SUBROUTINE = <string>subroutine_name | 
ELEMENT BLOCK SUBROUTINE = <string>subroutine_name 
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON 
SUBROUTINE REAL PARAMETER: <string>param_name
   = <real>param_value 
SUBROUTINE INTEGER PARAMETER: <string>param_name
   = <integer>param_value 
SUBROUTINE STRING PARAMETER: <string>param_name
   = <string>param_value 
{end command block}
```

A number of user subroutine command lines will appear in some Presto command block. User subroutine commands can appear in boundary condition, element death, user output, and state initialization command blocks. The possible command lines are shown above. The following sections describe the command lines related to user subroutines.

9.2.2.1 Type

User subroutines are currently available in three general types: node set, surface, and element.
Node set subroutines operate on groups of nodes. The command line for defining a node set subroutine is:

```
NODE SET SUBROUTINE = <string>subroutine_name
```

where `subroutine_name` is the name of the user subroutine. The name is case sensitive. A node set subroutine will operate on all nodes contained in an associated mechanics instance.

Surface subroutines work on groups of surfaces. A surface may be an external face of a solid element or the face of a shell element associated with either the positive or negative normal for the surface of the shell. The command line for defining a surface subroutine is:

```
SURFACE SUBROUTINE = <string>subroutine_name
```

Element block subroutines work on groups of elements. The command line for defining an element block subroutine is:

```
ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
```

An element may be a solid element such as a hexahedron or a two-dimensional element such as a shell.

Different Presto features may accept one or more types of user subroutines. Only one subroutine is allowed per command block.

### 9.2.2.2 Debugging

Subroutines may be run in a special debugging mode to help catch memory errors. For example, there is a potential for a user subroutine to write outside of its allotted data space by writing beyond the bounds of an input or output array. Generally, this causes Presto to crash, but it also has the potential to introduce other very hard-to-trace bugs into the Presto analysis. Subroutines run in debug mode require more memory and more processing time than subroutines not run in debug mode.

Subroutine debugging is on by default in debug executables. It can be turned off with the following command line:

```
SUBROUTINE DEBUGGING OFF
```

Subroutine debugging is off by default in optimized executables. It can be turned on with the following command line:

```
SUBROUTINE DEBUGGING ON
```

### 9.2.2.3 Parameters

All user subroutines have the ability to use parameters. Parameters are defined in the input file and are quickly accessible by the user subroutine during run time. Parameters are a way of making a single user subroutine much more versatile. For example, a user subroutine could be written to define a periodic loading on a structure. A parameter for the subroutine could be defined specifying the frequency of the function. In this way, the same subroutine can be used in different parts of
the model, and the subroutine behavior can be modified without recompiling the program. These command lines are placed within the scope of the command block in which the user subroutine is specified.

Real-valued parameters can be stored with the following command line:

```
SUBROUTINE REAL PARAMETER: <string>param_name = <real>param_value
```

Integer-valued parameters can be stored with the following command line:

```
SUBROUTINE INTEGER PARAMETER: <string>param_name = <integer>param_value
```

String-valued parameters can be stored with the following command line:

```
SUBROUTINE STRING PARAMETER: <string>param_name = <string>param_value
```

Any number of subroutine parameters may be defined. The subroutine parameters may be defined in any order within the command block. The user subroutine may request the values of the parameters but is not required to use them or even have any knowledge of their existence. An example of subroutine usage with parameters is as follows:

```
BEGIN PRESSURE
  SURFACE = surface_1
  SURFACE SUBROUTINE = blast_pressure
  SUBROUTINE REAL PARAMETER: blast_time = 1.2
  SUBROUTINE REAL PARAMETER: blast_power = 1.3e+07
  SUBROUTINE STRING PARAMETER: formulation = alpha
  SUBROUTINE INTEGER PARAMETER: decay_exponent = 2
  SUBROUTINE DEBUGGING ON
END PRESSURE
```

In the above example, four parameters are associated with the subroutine `blast_pressure`. Two of the parameters are real (`blast_time` and `blast_power`), one of the parameters is a string (`formulation`), and one of the parameters is an integer (`decay_exponent`). To access the parameters in the user subroutine, the user will need to include interface calls described in previous sections.
9.2.3 Time Step Initialization

BEGIN TIME STEP INITIALIZATION
  # mesh-entity set commands
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list> surface_names
  REMOVE BLOCK = <string list>block_names
  #
  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name |
  SURFACE SUBROUTINE = <string>sub_name |
  ELEMENT BLOCK SUBROUTINE = <string>sub_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
  #
  # additional command
  ACTIVE PERIODS = <string list>period_names
END TIME STEP INITIALIZATION

The TIME STEP INITIALIZATION command block, which appears in the region scope, is used to flag a user subroutine to run at the beginning of every time step. This subroutine can be used to compute quantities used by other command types. For example, if the traction on a surface was dependent on the area, the time step initialization subroutine could be used to calculate the area, and that area could be stored and later read when calculating the traction. The user initialization subroutine will pass the specified mesh objects to the subroutine for use in calculating some value.

The TIME STEP INITIALIZATION command block contains two groups of commands—mesh entity set and user subroutine. In addition to the command lines in these command groups, there is an additional command line: ACTIVE PERIODS. The ACTIVE PERIODS command line is used to activate or deactivate the running of the user subroutine at the beginning of every time step for certain time periods. Following are descriptions of the different command groups and the ACTIVE PERIODS command lines.

9.2.3.1 Mesh-Entity Set Commands

The mesh-entity set commands portion of the TIME STEP INITIALIZATION command block specifies the nodes, element faces, or elements associated with the particular subroutine that
will be run at the beginning of the applicable time steps. This portion of the command block can include some combination of the following command lines:

```
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list> surface_names
REMOVE BLOCK = <string list>block_names
```

These command lines, taken collectively, constitute a set of Boolean operators for constructing a set of nodes, element faces, or elements. See Section 5.1 for more information about the use of these command lines for mesh entities. There must be at least one NODE SET, SURFACE, BLOCK, or INCLUDE ALL BLOCKS command line in the command block.

### 9.2.3.2 User Subroutine Commands

The following command lines are related to the user subroutine specification:

```
NODE SET SUBROUTINE = <string>subroutine_name |
SURFACE SUBROUTINE = <string>subroutine_name |
ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
```

Only one of the first three command lines listed above can be specified in the command block. The particular command line selected depends on the mesh-entity type of the variable being initialized. For example, variables associated with nodes would be initialized if you are using the NODE SET SUBROUTINE command line, variables associated with faces if you are using the SURFACE SUBROUTINE command line, and variables associated with elements if you are using the ELEMENT BLOCK SUBROUTINE command line. The string subroutine_name is the name of a FORTRAN subroutine that is written by the user.

Following the selected subroutine command line are other command lines that may be used to implement the user subroutine option. These command lines are described in Section 9.2.2 and consist of SUBROUTINE DEBUGGING OFF, SUBROUTINE DEBUGGING ON, SUBROUTINE REAL PARAMETER, SUBROUTINE INTEGER PARAMETER, and SUBROUTINE STRING PARAMETER. Examples of using these command lines are provided throughout Chapter 9.
9.2.3.3 Additional Command

The `ACTIVE PERIODS` command line can optionally appear in the `TIME STEP INITIALIZATION` command block:

```
ACTIVE PERIODS = <string list>period_names
```

This command line determines when time step initialization by a user subroutine is active. See Section 2.5 for more information about this optional command line.
9.2.4 User Variables

BEGIN USER VARIABLE <string>var_name
    TYPE = <string>NODE|ELEMENT|GLOBAL
        [<string>REAL|INTEGER LENGTH = <integer>length]
        [<string>SYM_TENSOR|FULL_TENSOR|VECTOR]
    GLOBAL OPERATOR = <string>SUM|MIN|MAX
    INITIAL VALUE = <real list>values
    USE WITH RESTART
END [USER VARIABLE <string>var_name]

The **USER VARIABLE** command block is used to create a user-defined variable. This kind of variable may be used for scratch space in a user subroutine or for some user-defined output. A user-defined variable may be output to the results file or the history file just like any registered variable; i.e., a user-defined variable once defined by the **USER VARIABLE** command block can be specified in a **USER OUTPUT** command block, a **RESULTS OUTPUT** command block, and a **HISTORY OUTPUT** command block.

User-defined variables are associated with mesh entities. For example, a node variable will exist at every node of the model. An element variable will exist on every element of the model. A global variable will have a single value for the entire model.

If the user-defined variable functionality is used in conjunction with restart, the **USE WITH RESTART** command line must be included.

**Known Issue:** User defined variables are not currently supported with heartbeat output (see Section 8.3).

The **USER VARIABLE** command block is placed within a Presto region. The command block begins with the input line:

```
BEGIN USER VARIABLE <string>var_name
```

and ends with the input line:

```
END [USER VARIABLE <string>var_name]
```

where `var_name` is a user-selected name for the variable.

In the above command block:

- A user-defined variable has an associated type that is specified by the **TYPE** command line, which itself contains several parameters. The **TYPE** command line is required.

1. The variable must be a nodal quantity, an element quantity, or a global quantity. The options **NODE**, **ELEMENT**, and **GLOBAL** determine whether the variable will be a nodal, element, or global quantity. One of these options must appear on the **TYPE** command line.
2. The user-defined variable can be either an integer or a real, as specified by the INTEGER or REAL option.

3. The length of the variable must be set by using one of the options SYM_TENSOR, FULL_TENSOR, VECTOR, or LENGTH = <integer>length. If the LENGTH option is used, the user must specify whether the variable is an integer number or a real number by using the INTEGER or REAL option. If the SYM_TENSOR option is used, the variable has six real components. If the FULL_TENSOR is used, the variable has nine real components. If the VECTOR option is used, the variable has three real components. The three options SYM_TENSOR, FULL_TENSOR, and VECTOR all imply real numbers, and thus the REAL option need not be included in the command line when one of these three options is specified.

Some examples of the TYPE command line follow:

```plaintext
type = global real length = 1
type = element tensor
type = element real length = 3
type = node sym_tensor
type = node vector
```

- If you use the GLOBAL option on the TYPE command line, a global variable is created, and this global variable must be given an associated reduction type, which is specified by the GLOBAL OPERATOR command line. The reduction type tells Presto how to reduce the individual values stored on each processor to a mesh global value. Global reductions are performed at the end of each time step. Any modifications to a global variable made by an aupst_local_put_global_var call (see Section 9.1.2.5) will not be seen until the next time step after the user-defined global variables have been updated and reduced. The SUM operator sums all processor variable contributions. The MAX operator takes the maximum value of the aupst_local_put_global_var calls. The MIN operator takes the minimum value of the aupst_local_put_global_var calls.

- One or more initial values may be specified for the user-defined variable in the INITIAL VALUE command line. The number of initial values specified should be the same as the length of the variable, as specified in the TYPE command line either explicitly via the LENGTH option or implicitly via the SYM_TENSOR, FULL_TENSOR, or VECTOR option. The initial values will be copied to the variable space on every mesh object on which the variable is defined. Only real type variables may be given initial values at this time.

- All intrinsic type options such as REAL, INTEGER, SYM_TENSOR, FULL_TENSOR, VECTOR and the LENGTH option can be used with any of the mesh entity options (NODE, ELEMENT, GLOBAL).

- As indicated previously, if the user-defined variable functionality is used in conjunction with restart, the USE WITH RESTART command line must be included.
9.3 User Subroutines: Compilation and Execution

Running a code with user subroutines is a two-step process. First, you must create an executable version of Presto that recognizes the user subroutines. Next, you must use this version of Presto for an actual Presto run with an input file that incorporates the proper user subroutine command lines.

How the above two steps are carried out is site-specific. The actual process will depend on how Presto is set up at your installation. We will give an example that shows how the process is carried out on various systems at Sandia using SIERRA command lines. SIERRA is a general code framework and code management system at Sandia.

For the first step, you will need the user subroutine, in a FORTRAN file, and a Presto input file that makes use of the user subroutine. You will use a system command line of the general form shown below.

```
% sierra presto -i <string>input_file_name --make
```

Suppose that you have a subdirectory in your area called `test` and you wish to incorporate a user subroutine called `blast_load`. The actual user subroutine will be in a file called `blast_load.F`, and the associated input file will be called `blast_load_1.i`. Both of these files will be in the directory `test`. In the input file, you will have the following command line in the domain scope:

```
USER SUBROUTINE FILE = blast_load.F
```

You will also have some subset of the command lines described in the previous section in your Presto input file. The specific form of the system command line to execute the first step of the user subroutine process is shown below.

```
% sierra presto -i blast_load_1.i --make
```

The above command will create a local version of Presto in a local directory named `UserSubsProject`. The system command line to run the local version of Presto is shown below.

```
% sierra presto -i <string>input_file_name -x UserSubsProject
```

The specific form of the system command line you will execute in the subdirectory test is shown below.

```
% sierra presto -i blast_load_1.i -x UsersSubsProjects
```

The second command line runs Presto using `blast_load_1.i` as an input file and utilizes the user subroutines in the process. Again, all of this is a site-specific example. You must determine how Presto is set up at your installation to determine what system command lines are necessary to build Presto with user subroutines and then use this version of Presto.
9.4 User Subroutines: Examples

9.4.1 Pressure as a Function of Space and Time

(The following example provides functionality—a blast load on a surface—more applicable to Presto than Adagio. It is included in both manuals as it is instructive in the general use of a user-defined subroutine.)

The following code is an example of a user subroutine to compute blast pressures on a group of faces. The blast pressure simulates a blast occurring at a specified position and time. The blast wave radiates out from the center of the blast and dissipates over time. This subroutine is included in the input file as follows:

```fortran
# In the domain scope:
user subroutine file = blast_load.F

# In the region scope:
begin pressure
  surface = surface_1
  surface subroutine = blast_load
  subroutine real parameter: pos_x = 5.0
  subroutine real parameter: pos_y = 5.0
  subroutine real parameter: pos_z = 1.6
  subroutine real parameter: wave_speed = 1.5e+02
  subroutine real parameter: blast_time = 0.0
  subroutine real parameter: blast_energy = 1.0e+09
  subroutine real parameter: blast_wave_width = 0.75
end pressure
```

The FORTRAN 77 subroutine listing follows. Note that it would be possible to increase the speed of this subroutine by calling the topology functions (see Section 9.1.2.6) on groups of elements, though this would increase subroutine complexity.

```fortran
c
Subroutine to simulate a blast load on a surface

subroutine blast_load(num_faces, num_vals, & eval_time, faceID, pressure, flags, err_code)

  implicit none

Subroutine input arguments

c  integer num_faces
c  double precision eval_time
c  integer faceID(num_faces)
```
integer num_vals

c Subroutine output arguments

double precision pressure(num_vals, num_faces)
integer flags(num_faces)
integer err_code

c Variables to hold the subroutine parameters

double precision pos_x, pos_y, pos_z, wave_speed,
& blast_time, blast_energy,
& blast_wave_width

c Local variables

integer iface, inode
integer cur_face_id, face_topo, num_nodes
integer num_comp_check
double precision dist, blast_o_rad, blast_i_rad
double precision blast_volume, blast_pressure
integer query_error
double precision face_center(3)

c Create some static variables to hold queried information. Assume no face has more than 10 nodes

double precision face_nodes(10)
double precision face_coords(3, 10)

c Extract the subroutine parameters

call aupst_get_real_param("pos_x", pos_x, query_error)
call aupst_get_real_param("pos_y", pos_y, query_error)
call aupst_get_real_param("pos_z", pos_z, query_error)
call aupst_get_real_param("wave_speed", wave_speed,
& query_error)
call aupst_get_real_param("blast_energy",
& blast_energy, query_error)
call aupst_get_real_param("blast_time",
& blast_time, query_error)
call aupst_get_real_param("blast_wave_width",
& blast_wave_width, query_error)

c Determine the outer radius of the blast wave
\begin{verbatim}

blast_o_rad = (eval_time - blast_time) * wave_speed
if(blast_o_rad .le. 0.0) return;

Determine the inner radius of the blast wave

blast_i_rad = blast_o_rad - blast_wave_width
if(blast_i_rad .le. 0.0) blast_i_rad = 0.0

Determine the total volume the blast wave occupies

blast_volume = 3.1415 * (4.0/3.0) *
& (blast_o_rad**2 - blast_i_rad**2)

Determine the total pressure on faces inside the
blast wave

blast_pressure = blast_energy / blast_volume

Loop over all faces in the set

do iface = 1, num_faces

Extract the topology of the current face

cur_face_id = faceID(iface)
call aupst_get_face_topology(1, cur_face_id,
& face_topo, query_error)

Determine the number of nodes of the current face

num_nodes = mod(face_topo,100)

Extract the node ids for nodes contained in the current
face

call aupst_get_face_nodes(1, cur_face_id,
& face_nodes, query_error)

Extract the nodal coordinates of the face nodes

call aupst_get_node_var(num_nodes, 3, face_nodes,
& face_coords, "coordinates", query_error)

Compute the centroid of the face

face_center(1) = 0.0
\end{verbatim}
face_center(2) = 0.0
face_center(3) = 0.0
do inode = 1, num_nodes
    face_center(1) = face_center(1) + 
    & face_coords(1,inode)
    face_center(2) = face_center(2) + 
    & face_coords(2,inode)
    face_center(3) = face_center(3) + 
    & face_coords(3,inode)
enddo
face_center(1) = face_center(1)/num_nodes
face_center(2) = face_center(2)/num_nodes
face_center(3) = face_center(3)/num_nodes

c
Determine the distance from the current face

c to the blast center

c
dist = sqrt((face_center(1) - pos_x)**2 +
    & (face_center(2) - pos_y)**2 +
    & (face_center(3) - pos_z)**2)
c
Apply pressure to the current face if it falls within
the blast wave

c
    if(dist .ge. blast_i_rad .and.
    & dist .le. blast_o_rad) then
        pressure(1,iface) = blast_pressure
    else
        pressure(1,iface) = 0.0
    endif
endo
err_code = 0
end

9.4.2 Error Between a Computed and an Analytic Solution

The following code is a user subroutine to compute the error between Presto-computed results and results from an analytic manufactured solution. This subroutine is called by a USER OUTPUT command block immediately prior to producing an output Exodus file. The error for the mesh is computed by taking the squared difference between the computed and analytic displacements at every node. Finally, a global sum of the error is produced along with the square root norm of the error.

This user subroutine requires a user variable, which is defined in the Presto input file. The command block for the user variable specified in this user subroutine is as follows:

    begin user variable conv_error
type = global real length = 1
global operator = sum
initial value = 0.0
end user variable conv_error

The subroutine is called in the Presto input file as follows:

begin user output
node set = nodelist_10
node set subroutine = conv0_error
subroutine real parameter: char_length = 1.0
subroutine real parameter: char_time = 1.0e-3
subroutine real parameter: x_offset = 0.0
subroutine real parameter: y_offset = 0.0
subroutine real parameter: z_offset = 0.0
subroutine real parameter: t_offset = 0.0
subroutine real parameter: u0 = 0.01
subroutine real parameter: v0 = 0.02
subroutine real parameter: w0 = 0.03
subroutine real parameter: alpha = 1.0
subroutine real parameter: youngs_modulus = 10.0e6
subroutine real parameter: poissons_ratio = 0.3
subroutine real parameter: density = 0.0002588
subroutine real parameter: num_nodes = 125.0
end user output

The FORTRAN listing for the subroutine is as follows:

```fortran
subroutine conv0_error(num_nodes, num_vals,  
& eval_time, nodeID, values, flags, ierror)
  implicit none

  integer num_nodes
  integer num_vals
  double precision eval_time
  integer nodeID(num_nodes)
  double precision values(1)
  integer flags(1)
  integer ierror

  c
  c Local vars
  c

  integer inode
  integer error_code
  double precision clength, ctime, xoff, yoff, zoff, toff
  double precision zero, one, two, three, four, nine
```
double precision mod_coords(3,3000)
double precision cdispl(3,3000)
integer num_comp_check
double precision expat
double precision x, y, z, t
double precision u0, v0, w0, alpha
double precision pi
double precision half
double precision mdisplx, mdisply, mdisplz
double precision xdiff, ydiff, zdiff
double precision conv_error
double precision numnod

pi = 3.141592654
half = 0.5
zero = 0.0
one = 1.0
two = 2.0
three = 3.0
four = 4.0
nine = 9.0

c Check that the nodal coordinates will fit into the
c statically allocated array
c
if(num_nodes .gt. 3000) then
   write(6,*) 'ERROR in sphere disp, ', &
   & num_nodes exceeds static array size$
   ierror = 1
   return
endif
c
 Extract the model coordinates for all nodes
c
   call aupst_check_node_var(num_nodes, num_comp_check,
   & nodeID, "model_coordinates", &
   & ierror)
   if(ierror .ne. 0) return
   if(num_comp_check .ne. 3) return
   call aupst_get_node_var(num_nodes, num_comp_check,
   & nodeID, mod_coords, "model_coordinates", &
   & ierror)
c
 Extract the computed displacements for all nodes
c
   call aupst_check_node_var(num_nodes, num_comp_check,
   & nodeID, "displacement", &
& ierror)
if(ierror .ne. 0) return
if(num_comp_check .ne. 3) return
call aupst_get_node_var(num_nodes, num_comp_check,
& nodeID, cdispl, "displacement",
& ierror)

c Extract the subroutine parameters.
c
call aupst_get_real_param("char_length",
& clength,error_code)
call aupst_get_real_param("char_time",
& ctime,error_code)
call aupst_get_real_param("x_offset",xoff,error_code)
call aupst_get_real_param("y_offset",yoff,error_code)
call aupst_get_real_param("z_offset",zoff,error_code)
call aupst_get_real_param("t_offset",toff,error_code)
call aupst_get_real_param("u0",u0,error_code)
call aupst_get_real_param("v0",v0,error_code)
call aupst_get_real_param("w0",w0,error_code)
call aupst_get_real_param("alpha",alpha,error_code)
call aupst_get_real_param("num_nodes",
& numnod,error_code)

c Calculate a solution scaling factor
c
expat = half * ( one - cos( pi * eval_time / ctime ) )
c Compute the expected solution at each node and do a
c sum of the differences from the analytic solution
c
conv_error = zero
do inode = 1, num_nodes
c
Set the displacement value from the manufactured solution
c
x = ( mod_coords(1,inode) - xoff ) / clength
y = ( mod_coords(2,inode) - yoff ) / clength
z = ( mod_coords(3,inode) - zoff ) / clength

mdisplx = u0 * sin(x) * cos(two*y) * cos(three*z)
* * expat
mdisply = v0 * cos(three*x) * sin(y) * cos(two*z)
* * expat
mdisplz = w0 * cos(two*x) * cos(three*y) * sin(z)
* * expat
9.4. USER SUBROUTINES: EXAMPLES

\[
\begin{align*}
\text{xdiff} &= m\text{displx} - c\text{displ}(1,\text{inode}) \\
\text{ydiff} &= m\text{disply} - c\text{displ}(2,\text{inode}) \\
\text{zdiff} &= m\text{displz} - c\text{displ}(3,\text{inode}) \\
\text{conv\_error} &= \text{conv\_error} + \text{xdiff} \times \text{xdiff} \\
&\quad + \text{ydiff} \times \text{ydiff} \\
&\quad + \text{zdiff} \times \text{zdiff}
\end{align*}
\]

```c
ierror = 0

c
Do a parallel sum of the squared errors and extract the total summed value on all processors

call aupst_put_global_var(1, conv_error, &"conv_error","sum",ierror)
call aupst_get_global_var(1, conv_error, &"conv_error",ierror)

c
Take the square root of the errors and store that as the net error norm

cconv_error = sqrt(conv_error) / sqrt(numnod)
call aupst_put_global_var(1, conv_error, &"conv_error","none",ierror)

creturn
cend
```

9.4.3 Transform Output Stresses to a Cylindrical Coordinate System

The following code is a user subroutine to transform element stresses in global \(x\), \(y\), and \(z\) coordinates to a global cylindrical coordinate system. This subroutine could be used to transform the relatively meaningless shell stress in \(x\), \(y\), and \(z\) coordinates to more meaningful tangential, hoop, and radial stresses. The subroutine is called from a USER OUTPUT command block. It reads in the old stresses, transforms them, and writes them back out to a user-created scratch variable, defined via a USER VARIABLE command block, for output.

begin user variable cyl_stress
  type = element sym_tensor length = 1
  initial value = 0.0 0.0 0.0 0.0 0.0 0.0
end user variable

begin user output
  block = block_1
  element block subroutine = aupst_cyl_transform
subroutine string parameter: origin_point = Point_O
subroutine string parameter: z_point = Point_Z
subroutine string parameter: xz_point = Point_XZ
subroutine string parameter: input_stress = memb_stress
subroutine string parameter: output_stress = cyl_stress
end user output

The FORTRAN listing for the subroutine is as follows:

```fortran
subroutine aupst_cyl_transform(num_elems, num_vals,
* eval_time, elemID, values, flags, ierror)
  implicit none
  #include<framewk/Fmwk_type_sizes_decl.par>
  #include<framewk/Fmwk_type_sizes.par>
  c
  c Subroutine Arguments
  c
  c num_elems: Input: Number of elements to calculate on
  c num_vals : Input: Ignored
  c eval_time: Input: Time at which to evaluate the stress.
  c elemID : Input: Global sierra IDs of the input elements
  c values : I/O : Ignored, stress will be stored manually
  c flags : I/O : Ignored
  c ierror : Output: Returns non-zero if an error occurs
  c
  integer num_elems
  integer num_vals
  double precision eval_time
  integer elemID(num_elems)
  double precision values(1)
  integer flags(1)
  integer ierror
  
  c Fortran cannot dynamically allocate memory, thus worksets
c will be iterated over by chunks each of size chunk_size.
  c
  integer chunk_size
  parameter (chunk_size = 100)
  integer chunk_ids(chunk_size)
  
  c Subroutine parameter data
  c
  character*80 origin_point_name
  double precision origin_point(3)
  character*80 z_point_name
  double precision z_point(3)
  character*80 xz_point_name
```
double precision xz_point(3)
character*80 input_stress_name
character*80 output_stress_name

c Local element data for centroids and rotation vectors
c
double precision cent(3)
double precision centerline_pos(3)
double precision dot_prod
double precision z_vec(3)
double precision r_vec(3)
double precision theta_vec(3)
double precision rotation_tensor(9)

c Chunk data storage
c
double precision elem_centroid(3, chunk_size)
double precision input_stress_val(6, chunk_size)
double precision output_stress_val(6, chunk_size)

c Simple iteration variables
c
integer error_code
integer ichunk, ielem
integer zero_elem, nel

c Extract the current subroutine parameters. origin_point
c is the origin of the coordinate system
c z_point is a point on the z axis of the coordinate system
c xz_point is a point on the xz plane
c
    call aupst_get_string_param("origin_point",
    &     origin_point_name,
    &     error_code)
    call aupst_get_string_param("z_point",
    &     z_point_name,
    &     error_code)
    call aupst_get_string_param("xz_point",
    &     xz_point_name,
    &     error_code)
    call aupst_get_string_param("input_stress",
    &     input_stress_name,
    &     error_code)
    call aupst_get_string_param("output_stress",
    &     output_stress_name,
    &     error_code)


c Use the point names to look up the coordinates of each relevant point
c
    call aupst_get_point(origin_point_name, origin_point, &
                          error_code)
    call aupst_get_point(z_point_name, z_point, &
                          error_code)
    call aupst_get_point(xz_point_name, xz_point, &
                          error_code)

c Compute the z axis vector
c
    z_vec(1) = z_point(1) - origin_point(1)
    z_vec(2) = z_point(2) - origin_point(2)
    z_vec(3) = z_point(3) - origin_point(3)

c Transform z_vec into a unit vector, abort if it is invalid
c
    call aupst_unitize_vector(z_vec, ierror)
    if(ierror .ne. 0) return

c Loop over chunks of the data arrays
c
    do ichunk = 1, (num_elems/chunk_size + 1)

c Determine the first and last element number for the current chunk of elements
c
    zero_elem = (ichunk-1) * chunk_size
    if((zero_elem + chunk_size) .gt. num_elems) then
        nel = num_elems - zero_elem
    else
        nel = chunk_size
    endif

c Copy the elemIDs for all elems in the current chunk to a temporary array
c
    do ielem = 1, nel
        chunk_ids(ielem) = elemID(zero_elem + ielem)
    enddo

c Extract the element centroids and stresses
c
    call aupst_get_elem_centroid(nel, chunk_ids, &
                                 elem_centroid,
                                 &
                                 ierror)
call aupst_get_elem_var(nel, 6, chunk_ids, 
& input_stress_val, 
& input_stress_name, ierror)

c Loop over each element in the current chunk
do ielem = 1, nel
c Find the closest point on the cylinder centerline axis
to the element centroid
cent(1) = elem_centroid(1, ielem) - origin_point(1)
cent(2) = elem_centroid(2, ielem) - origin_point(2)
cent(3) = elem_centroid(3, ielem) - origin_point(3)
dot_prod = cent(1) * z_vec(1) +
& cent(2) * z_vec(2) +
& cent(3) * z_vec(3)
centerline_pos(1) = z_vec(1) * dot_prod
centerline_pos(2) = z_vec(2) * dot_prod
centerline_pos(3) = z_vec(3) * dot_prod

c Compute the current normal radial vector
c_r_vec(1) = cent(1) - centerline_pos(1)
r_vec(2) = cent(2) - centerline_pos(2)
r_vec(3) = cent(3) - centerline_pos(3)
call aupst_unitize_vector(r_vec, ierror)
if(ierr .ne. 0) return

c Compute the current hoop vector
c theta_vec(1) = z_vec(2)*r_vec(3) - r_vec(2)*z_vec(3)
theta_vec(2) = z_vec(3)*r_vec(1) - r_vec(3)*z_vec(1)
theta_vec(3) = z_vec(1)*r_vec(2) - r_vec(1)*z_vec(2)
c The r, theta, and z vectors describe the new stress
c coordinate system. Transform the input stress tensor
in x,y,z coords to the output stress tensor in r, theta,
c and z coords use the unit vectors to create a rotation
tensor
c rotation_tensor(k_f36xx) = r_vec(1)
rotation_tensor(k_f36yx) = r_vec(2)
rotation_tensor(k_f36zx) = r_vec(3)
rotation_tensor(k_f36xy) = theta_vec(1)
rotation_tensor(k_f36yy) = theta_vec(2)
rotation_tensor(k_f36zy) = theta_vec(3)
rotation_tensor(k_f36xz) = z_vec(1)
rotation_tensor(k_f36yz) = z_vec(2)
rotation_tensor(k_f36zz) = z_vec(3)

c c Rotate the current stress tensor to the new configuration
   c
   call fmth_rotate_symten33(1, 1, 0, rotation_tensor,
                        & input_stress_val(1,ielem),
                        & output_stress_val(1,ielem))
   enddo

c c Store the new stress
   c
   call aupst_put_elem_var(nel, 6, chunk_ids,
                        & output_stress_val,
                        & output_stress_name, ierror)
   enddo
   ierror = 0
end
9.5 User Subroutines: Library

A number of user subroutines are used commonly and have been permanently incorporated into the code. These subroutines are used just like any other subroutines, but they do not need to be compiled into the code. (The user need be concerned only about the Presto command lines.) This section describes the usage of each of these subroutines.

9.5.1 aupst_cyl_transform

Author: Nathan Crane

Purpose:
The purpose of this subroutine is to transform element stresses from a global rectangular coordinate system to a local cylindrical coordinate system. This subroutine is generally called by a USER OUTPUT command block. For example:

```plaintext
begin user output
  block = block_1
  element block subroutine = aupst_cyl_transform
  subroutine string parameter: origin_point = Point_O
  subroutine string parameter: z_point = Point_Z
  subroutine string parameter: xz_point = Point_XZ
  subroutine string parameter: input_stress = memb_stress
  subroutine string parameter: output_stress = cyl_stress
end user output
```

Requirements:
This subroutine requires a tensor variable to store the cylindrical stress into a registered variable for each element. The registered variable is created by the following command block in the Presto region:

```plaintext
begin user variable cyl_stress
  type = element sym_tensor length = 1
  initial value = 0.0 0.0 0.0 0.0 0.0 0.0
end user variable
```
Parameters:

<table>
<thead>
<tr>
<th>Parameter Name</th>
<th>Usage</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>origin_point</td>
<td>String</td>
<td>Name of the point at the cylinder origin.</td>
</tr>
<tr>
<td>z_point</td>
<td>String</td>
<td>Point on the cylinder axis.</td>
</tr>
<tr>
<td>xz_point</td>
<td>String</td>
<td>Point on the line that passes through theta = 0 on the cylinder.</td>
</tr>
<tr>
<td>input_stress</td>
<td>String</td>
<td>Name of the Presto internal input stress tensor variable.</td>
</tr>
<tr>
<td>output_stress</td>
<td>String</td>
<td>Name of the Presto internal output stress tensor variable.</td>
</tr>
</tbody>
</table>

9.5.2 aupst_rec_transform

Author: Daniel Hammerand

Purpose:
The purpose of this subroutine is to transform element stresses from a global rectangular coordinate system to a different local rectangular coordinate system. This subroutine is generally called by a USER OUTPUT command block. For example:

```plaintext
begin user output
  block = block_1
  element block subroutine = aupst_rec_transform
  subroutine string parameter: origin_point = Point_O
  subroutine string parameter: z_point = Point_Z
  subroutine string parameter: xz_point = Point_XZ
  subroutine string parameter: input_stress = memb_stress
  subroutine string parameter: output_stress = new_stress
end user output
```

Requirements:
This subroutine requires a tensor variable to store the new stress into a registered variable for each element. The registered variable is created by the following command block in the Presto region:

```plaintext
begin user variable new_stress
  type = element sym_tensor length = 1
  initial value = 0.0 0.0 0.0 0.0 0.0 0.0
end user variable
```
Parameters:

<table>
<thead>
<tr>
<th>Parameter Name</th>
<th>Usage</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>origin_point</td>
<td>String</td>
<td>Name of the point at the cylinder origin.</td>
</tr>
<tr>
<td>z_point</td>
<td>String</td>
<td>Point on the cylinder axis.</td>
</tr>
<tr>
<td>xz_point</td>
<td>String</td>
<td>Point on the line that passes through theta = 0 on the cylinder.</td>
</tr>
<tr>
<td>input_stress</td>
<td>String</td>
<td>Name of the Presto internal input stress tensor variable.</td>
</tr>
<tr>
<td>output_stress</td>
<td>String</td>
<td>Name of the Presto internal output stress tensor variable.</td>
</tr>
</tbody>
</table>
Chapter 10

Example Problem

This chapter provides an example problem to illustrate the construction of an input file for an analysis. The example problem consists of 124 spheres made of lead enclosed in a steel box. The steel box has an open top into which a steel plate is placed (see Figure 10.1). A prescribed velocity is then applied on the steel plate, pushing it into the box and crushing the spheres contained within using frictionless contact. This problem is a severe test for the contact algorithms as the spheres crush into a nearly solid block. See Figure 10.2 for results of this problem.

![Figure 10.1: Mesh for example problem: (a) box (red and green surfaces) with plate in top (blue surface) and (b) mesh with blue and green surfaces removed to show internal spheres (yellow) with initial crush.](image)

The input file is described below, with comments to explain every few lines. Following the description, the full input file is listed again. Most of the key words in this example are all lowercase, which is different from the convention we have used to describe the command lines in this document. However, all the lowercase usage in the following example is an acceptable format in Presto.

The input file starts with a begin sierra statement (i.e., the first line of the SIERRA command block), as is required for all input files:

```
begin sierra crush_124_spheres
```
CHAPTER 10. EXAMPLE PROBLEM

(a) Additional Crush of Spheres
(b) Final Deformed Configuration

Figure 10.2: Mesh with blue and green surfaces removed to show internal spheres (yellow) after initial crush shown in Figure 10.1 (b).

We now need to define the functions used with this problem. The boundary conditions require a function for the initial velocity, as follows:

begin definition for function constant_velocity
    type is piecewise linear
    ordinate is velocity
    abscissa is time
    begin values
        0.0 30.0
        1.0 30.0
    end values
end definition for function constant_velocity

To define the boundary conditions, we need to define the direction for the initial velocity—this is in the y-direction. We could also choose to simply specify the Y component for the initial condition, but this input file uses directions.

define direction y_axis with vector 0.0 1.0 0.0

Next we define the material models that will be used for this analysis. There are two materials in this problem: steel for the box, and lead for the spheres. Both materials use the elastic-plastic material model (denoted as elastic_plastic).

begin property specification for material steel
    density = 7871.966988

    begin parameters for model elastic_plastic
        youngs modulus = 1.999479615e+11
        poissons ratio = 0.33333
        yield stress = 275790291.7
        hardening modulus = 275790291.7
    end parameters
end property specification for material steel
beta = 1.0
end parameters for model elastic_plastic
end property specification for material steel

begin property specification for material lead
density = 11253.30062

begin parameters for model elastic_plastic
youngs modulus = 1.378951459e+10
poissons ratio = 0.44
yield stress = 13789514.59
hardening modulus = 0.0
beta = 1.0
end parameters for model elastic_plastic
end property specification for material lead

Now we define the finite element mesh. This includes specification of the file that contains the
mesh, as well as a list of all the element blocks we will use from the mesh and the material
associated with each block. The name of the file is crush_124_spheres.g. The specification
of the database type is optional—ExodusII is the default. Currently, each element block must be
defined individually. For this particular problem, all the spheres are the same element block. Each
sphere is a distinct geometry entity, but all spheres constitute one element block in the Exodus II
database. Note that the three element blocks that make up the box and lid all reference the same
material description. The material description is not repeated three times. The material description
for steel appears once and is then referenced three times.

begin finite element model mesh1
Database Name = crush_124_spheres.g
Database Type = exodusII

begin parameters for block block_1
material linear_elastic_steel
solid mechanics use model elastic_plastic
end parameters for block block_1

begin parameters for block block_2
material linear_elastic_steel
solid mechanics use model elastic_plastic
end parameters for block block_2

begin parameters for block block_3
material linear_elastic_steel
solid mechanics use model elastic_plastic
end parameters for block block_3
begin parameters for block block_4
    material linear_elastic_lead
    solid mechanics use model elastic_plastic
end parameters for block block_4

end finite element model mesh1

As an alternative to referencing the material description for steel three times as done above, you could define multiple element blocks simultaneously on the same command line. Thus, the three element block specifications with the material linear_elastic_steel could be consolidated into one, as follows:

begin parameters for block block_1 block 2 block 3
    material linear_elastic_steel
    solid mechanics use model elastic_plastic
end parameters for block block_1 block 2 block 3

At this point we have finished specifying physics-independent quantities. We now want to set up the Presto procedure and region, along with the time control command block. We start by defining the beginning of the procedure scope, the time control command block, and the beginning of the region scope. Only one time stepping block command block is needed for this analysis. The termination time is set to $7 \times 10^{-4}$.

begin presto procedure Apst_Procedure

begin time control
    begin time stepping block p1
        start time = 0.0
        begin parameters for presto region presto
            time step scale factor = 1.0
            time step increase factor = 2.0
            step interval = 25
        end parameters for presto region presto
    end time stepping block p1

termination time = 7.0e-4
end time control

begin presto region presto

Next we associate the finite element model we defined above (mesh1) with this presto region.

use finite element model model mesh1
Now we define the boundary conditions on the problem. We prescribe the velocity on the top surface of the box (nodelist_100) to crush the spheres, and we confine the bottom surface of the box (nodelist_200) not to move. Note that although we use node sets to define these boundary conditions, we could have used the corresponding side sets.

\begin{verbatim}
begin prescribed velocity
  node set = nodelist_100
  direction = y_axis
  function = constant_velocity
  scale factor = -1.0
end

begin fixed displacement
  node set = nodelist_200
  components = Y
end
\end{verbatim}

Now we define the contact for this problem. For this problem, we want all four element blocks to be able to contact each other, with a normal tolerance of 0.0001 and a tangential tolerance of 0.0005. In this case, we simply define the same contact characteristics for all interactions. However, we could also specify tolerances and kinematic partition factors for individual interactions. Since no friction model is defined in the block below, the contact defaults to frictionless contact. (There are numerous options you can use to control the contact algorithm. The options you choose will affect contact algorithm efficiency and solution accuracy. Consult with Chapter 7 to determine how to set input for the CONTACT DEFINITION command block to obtain the best level of efficiency and accuracy for your particular problem.)

\begin{verbatim}
begin contact definition
  skin all blocks = on
  begin search options
    normal tolerance = 0.0001
    tangential tolerance = 0.00005
  end
  begin interaction defaults
    general contact = on
    self contact = on
  end
end
\end{verbatim}

Now we define what variables we want in the results file, as well as how often we want this file to be written. Here we request files written every $7 \times 10^{-6}$ sec of analysis time. This will result in results output at one hundred time steps (plus the zero time step) since the termination time is set to $7 \times 10^{-4}$ sec. The output file will be called crush_124_spheres.e, and it will be an Exodus II file (the database type command is optional; it defaults to ExodusII). The variables we are requesting are the displacements and external forces at the nodes, the rotated stresses for the elements, the time-step increment, and the kinetic energy.
begin Results Output output_presto
Database Name = crush_124_spheres.e
Database Type = exodusII
At Time 0.0, Increment = 7.0e-6
  nodal Variables = displacement as displ
  nodal Variables = force_external as fext
  element Variables = rotated_stress as stress
  global Variables = KineticEnergy as KE
  global Variables = timestep
end

Now we end the presto region, presto procedure, and sierra blocks to complete the input file.

end presto region presto
end presto procedure Apst_Procedure
end sierra crush_124_spheres

Here is the resulting full input file for this problem:
begin sierra crush_124_spheres
begin definition for function constant_velocity
  type is piecewise linear
  ordinate is velocity
  abscissa is time
  begin values
    0.0 30.0
    1.0 30.0
  end values
end definition for function constant_velocity
define direction y_axis with vector 0.0 1.0 0.0

begin property specification for material steel
  density = 7871.966988

  begin parameters for model elastic_plastic
    youngs modulus = 1.999479615e+11
    poissons ratio = 0.33333
    yield stress = 275790291.7
    hardening modulus = 275790291.7
    beta = 1.0
  end parameters for model elastic_plastic
end property specification for material steel

begin property specification for material lead
  density = 11253.30062

  begin parameters for model elastic_plastic
    youngs modulus = 1.378951459e+10
    poissons ratio = 0.44
    yield stress = 13789514.59
    hardening modulus = 0.0
    beta = 1.0
  end parameters for model elastic_plastic
end property specification for material lead

begin finite element model mesh1
  Database Name = crush_124_spheres.g
  Database Type = exodusII

  begin parameters for block block_1
    material linear_elastic_steel
    solid mechanics use model elastic_plastic
  end parameters for block block_1
begin parameters for block block_2
  material linear_elastic_steel
  solid mechanics use model elastic_plastic
end parameters for block block_2

begin parameters for block block_3
  material linear_elastic_steel
  solid mechanics use model elastic_plastic
end parameters for block block_3

begin parameters for block block_4
  material linear_elastic_lead
  solid mechanics use model elastic_plastic
end parameters for block block_4

end finite element model mesh1

begin presto procedure Apst_Procedure

begin time control
  begin time stepping block p1
    start time = 0.0
    begin parameters for presto region presto
      time step scale factor = 1.0
      time step increase factor = 2.0
      step interval = 25
    end parameters for presto region presto
  end time stepping block p1

  termination time = 7.0e-4
end time control

begin presto region presto

  use finite element model mesh1

  begin prescribed velocity
    node set = nodelist_100
    direction = y_axis
    function = constant_velocity
    scale factor = -1.0
  end prescribed velocity

  begin fixed displacement
    node set = nodelist_200
    components = Y
  end fixed displacement
begin contact definition
  skin all blocks = on
  begin search options
    normal tolerance = 0.0001
    tangential tolerance = 0.00005
  end
  begin interaction defaults
    general contact = on
    self contact = on
  end
end

begin Results Output output_presto
  Database Name = crush_124_spheres.e
  Database Type = exodusII
  At Time 0.0, Increment = 7.0e-6
  nodal Variables = displacement as displ
  nodal Variables = force_external as fext
  element Variables = rotated_stress as stress
  global Variables = KineticEnergy as KE
  global Variables = timestep
end results output output_presto

end presto region presto
end presto procedure Apst_Procedure
end sierra crush_124_spheres
Chapter 11

Command Summary

This chapter gives all of the Presto commands in the proper scope.

# Domain specification
BEGIN SIERRA <string>name

# Title
TITLE = <string list>title

# Restart time
RESTART TIME = <real>restart_time
RESTART = AUTOMATIC

# User subroutine file
USER SUBROUTINE FILE = <string>file name

# Function definition
BEGIN DEFINITION FOR FUNCTION <string>function_name
    TYPE = <string>CONSTANT|PIECEWISE LINEAR| ANALYTIC
    ABSCISSA = <string>abscissa_label
    ORDINATE = <string>ordinate_label
    BEGIN VALUES
        <real>value_1 [<real>value_2
        <real>value_3 <real>value_4
        ...
        <real>value_n]
    END [VALUES]
    EVALUATE EXPRESSION = <string>analytic_expression1;
                        analytic_expression2;...
END [DEFINITION FOR FUNCTION <string>function_name]
# Definitions

DEFINE POINT <string>point_name WITH COORDINATES
   <real>value_1 <real>value_2 <real>value_3

DEFINE DIRECTION <string>direction_name WITH VECTOR
   <real>value_1 <real>value_2 <real>value_3

DEFINE AXIS <string>axis_name WITH POINT
   <string>point_1 POINT <string>point_2

DEFINE AXIS <string>axis_name WITH POINT
   <string>point_name DIRECTION <string>direction

# Local coordinate system

BEGIN ORIENTATION <string>orientation_name
   SYSTEM = <string>RECTANGULAR|Z RECTANGULAR|CYLINDRICAL|SPHERICAL(RECTANGULAR)
   #
   POINT A = <real>global_ax <real>global_ay <real>global_az
   POINT B = <real>global_bx <real>global_by <real>global_bz
   #
   ROTATION ABOUT <integer> 1|2|3(1) = <real>theta(0.0)
END [ORIENTATION <string>orientation_name]

# Error estimator controller

BEGIN ERROR ESTIMATION CONTROLLER <string>err_name
   ERROR ESTIMATOR = <string>DISTORTION
   COMPUTE METRIC = <string>ASPECT_RATIO/SOLID_ANGLE/PERIMETER_RATIO
   COMPUTE STEP INTERVAL = <integer>step_int
   COMPUTE AT OUTPUT
END [ERROR ESTIMATION CONTROLLER <string>name]

# Rigid bodies

BEGIN RIGID BODY <string>rb_name
   MASS = <real>mass
   MASS LOCATION = <real>CGx <real>CGy <real>CGz
   INERTIA = <real>Ixx <real>Iyy <real>Izz <real>Ixy
            <real>Iyz <real>Izx
   POINT INERTIA = <real>Ixx <real>Iyy <real>Izz <real>Ixy
                <real>Iyz <real>Izx
   MAGNITUDE = <real>magnitude_of_velocity
DIRECTION = <string>direction_definition
ANGULAR VELOCITY = <real>omega
CYLINDRICAL AXIS = <string>axis_definition
END [RIGID BODY <string>rb_name]

# Elastic material

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
   <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
   <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
   <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL ELASTIC
   YOUNGS MODULUS = <real>youngs_modulus
   POISSONS RATIO = <real>poissons_ratio
   SHEAR MODULUS = <real>shear_modulus
   BULK MODULUS = <real>bulk_modulus
   LAMBDA = <real>lambda
END [PARAMETERS FOR MODEL ELASTIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Elastic fracture material

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
   <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
   <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
   <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL ELASTIC_FRACTURE
   YOUNGS MODULUS = <real>youngs_modulus
   POISSONS RATIO = <real>poissons_ratio
CHAPTER 11. COMMAND SUMMARY

SHEAR MODULUS = <real>shear_modulus
BULK MODULUS = <real>bulk_modulus
LAMBDA = <real>lambda
MAX STRESS = <real>max_stress
CRITICAL STRAIN = <real>critical_strain
END [PARAMETERS FOR MODEL ELASTIC_FRACTURE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Elastic-plastic material

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
  <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
  <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
  <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL ELASTIC_PLASTIC
YOUNGS MODULUS = <real>younsgs_modulus
POISSONS RATIO = <real>poissons_ratio
SHEAR MODULUS = <real>shear_modulus
BULK MODULUS = <real>bulk_modulus
LAMBDA = <real>lambda
YIELD STRESS = <real>yield_stress
HARDENING MODULUS = <real>hardening_modulus
BETA = <real>beta_parameter(1.0)
END [PARAMETERS FOR MODEL ELASTIC_PLASTIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Elastic-plastic power-law hardening

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
  <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
  <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
<string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL EP_POWER_HARD
  YOUNGS MODULUS = <real>youngs_modulus
  POISSONS RATIO = <real>poissons_ratio
  SHEAR MODULUS = <real>shear_modulus
  BULK MODULUS = <real>bulk_modulus
  LAMBDA = <real>lambda
  YIELD STRESS = <real>yield_stress
  HARDENING CONSTANT = <real>hardening_constant
  HARDENING EXPONENT = <real>hardening_exponent
  LUDERS STRAIN = <real>luders_strain
END [PARAMETERS FOR MODEL EP_POWER_HARD]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Elastic plastic power-law hardening with failure

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  #
  # {thermal strain option}
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
      <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
      <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
      <string>thermal_strain_z_function
  #
BEGIN PARAMETERS FOR MODEL DUCTILE_FRACTURE
  YOUNGS MODULUS = <real>youngs_modulus
  POISSONS RATIO = <real>poissons_ratio
  SHEAR MODULUS = <real>shear_modulus
  BULK MODULUS = <real>bulk_modulus
  LAMBDA = <real>lambda
  YIELD STRESS = <real>yield_stress
  HARDENING CONSTANT = <real>hardening_constant
  HARDENING EXPONENT = <real>hardening_exponent
  LUDERS STRAIN = <real>luders_strain
  CRITICAL TEARING PARAMETER = <real>crit_tearing
  CRITICAL CRACK OPENING STRAIN = <real>crit_crack
END [PARAMETERS FOR MODEL DUCTILE_FRACTURE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Multilinear elastic plastic power-law hardening
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
  <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
  <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
  <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL MULTILINEAR_EP
  YOUNGS MODULUS = <real>youngs_modulus
  POISSONS RATIO = <real>poissons_ratio
  SHEAR MODULUS = <real>shear_modulus
  BULK MODULUS = <real>bulk_modulus
  LAMBDA = <real>lambda
  YIELD STRESS = <real>yield_stress
  BETA = <real>beta_parameter(1.0)
  HARDENING FUNCTION = <real>hardening_function_name
  YOUNGS MODULUS FUNCTION = <real>ym_function_name
  POISSONS RATIO FUNCTION = <real>pr_function_name
  YIELD STRESS FUNCTION =
    <real>yield_stress_function_name
END [PARAMETERS FOR MODEL MULTILINEAR_EP]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
#
Multilinear elastic plaster power-law hardening with
# failure

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
  <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
  <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
  <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL ML_EP_FAIL
YOUNGS MODULUS = <real>youngs_modulus
POISSONS RATIO = <real>poissons_ratio
SHEAR MODULUS = <real>shear_modulus
BULK MODULUS = <real>bulk_modulus
LAMBDA = <real>lambda
YIELD STRESS = <real>yield_stress
BETA = <real>beta_parameter(1.0)
HARDENING FUNCTION = <real>hardening_function_name
YOUNGS MODULUS FUNCTION = <real>ym_function_name
POISSONS RATIO FUNCTION = <real>pr_function_name
YIELD STRESS FUNCTION =
  <real>yield_stress_function_name
CRITICAL TEARING PARAMETER = <real>crit_tearing
CRITICAL CRACK OPENING STRAIN = <real>crit_crack

END [PARAMETERS FOR MODEL ML_EP_FAIL]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# BCJ plasticity

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  #
  # {thermal strain option}
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
BEGIN PARAMETERS FOR MODEL BCJ
  YOUNGS MODULUS = <real>youngs_modulus
  POISSONS RATIO = <real>poissons_ratio
  SHEAR MODULUS = <real>shear_modulus
  BULK MODULUS = <real>bulk_modulus
  LAMBDA = <real>lambda
  C1 = <real>c1
  C2 = <real>c2
  C3 = <real>c3
  C4 = <real>c4
  C5 = <real>c5
  C6 = <real>c6
  C7 = <real>c7
  C8 = <real>c8
  C9 = <real>c9
C10 = <real>c10
C11 = <real>c11
C12 = <real>c12
C13 = <real>c13
C14 = <real>c14
C15 = <real>c15
C16 = <real>c16
C17 = <real>c17
C18 = <real>c18
C19 = <real>c19
C20 = <real>c20
DAMAGE EXPONENT = <real>damage_exponent
INITIAL ALPHA_XX = <real>alpha_xx
INITIAL ALPHA_YY = <real>alpha_yy
INITIAL ALPHAZZ = <real>alpha_zz
INITIAL ALPHA_XY = <real>alpha_xy
INITIAL ALPHA_YZ = <real>alpha_yz
INITIAL ALPHA_XZ = <real>alpha_xz
INITIAL KAPPA = <real>initial_kappa
INITIAL DAMAGE = <real>initial_damage
YOUNGS MODULUS FUNCTION = <string>ym_function_name
POISSONS RATIO FUNCTION = <string>pr_function_name
SPECIFIC HEAT = <real>specific_heat
THETA OPT = <integer>theta_opt
FACTOR = <real>factor
RHO = <real>rho
TEMP0 = <real>temp0
END [PARAMETERS FOR MODEL BCJ]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Soil and crushable foam

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  #
  # (thermal strain option)
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL SOIL_FOAM
  YOUNGS MODULUS = <real>youngs_modulus
POISSONS RATIO = <real>poissons_ratio
SHEAR MODULUS = <real>shear_modulus
BULK MODULUS = <real>bulk_modulus
LAMBDA = <real>lambda
A0 = <real>const_coeff_yieldsurf
A1 = <real>lin_coeff_yieldsurf
A2 = <real>quad_coeff_yieldsurf
PRESSURE CUTOFF = <real>pressure_cutoff
PRESSURE FUNCTION = <string>function_press_volstrain
END [PARAMETERS FOR MODEL SOIL_FOAM]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Foam plasticity

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  #
  # {thermal strain option}
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL FOAM_PLASTICITY
    YOUNGS MODULUS = <real>youngs_modulus
    POISSONS RATIO = <real>poissons_ratio
    SHEAR MODULUS = <real>shear_modulus
    BULK MODULUS = <real>bulk_modulus
    LAMBDA = <real>lambda
    PHI = <real>phi
    SHEAR STRENGTH = <real>shear_strength
    SHEAR HARDENING = <real>shear_hardening
    SHEAR EXponent = <real>shear_exponent
    HYDRO STRENGTH = <real>hydro_strength
    HYDRO HARDENING = <real>hydro_hardening
    HYDRO EXponent = <real>hydro_exponent
    BETA = <real>beta
  END [PARAMETERS FOR MODEL FOAM_PLASTICITY]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Elastic three-dimensional orthotropic
BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
BEGIN PARAMETERS FOR MODEL ELASTIC_3D_ORTHOTROPIC
YOUNGS MODULUS AA = <real>Eaa_value
YOUNGS MODULUS BB = <real>Ebb_value
YOUNGS MODULUS CC = <real>Ecc_value
POISSONS RATIO AB = <real>NUab_value
POISSONS RATIO BC = <real>NUbc_value
POISSONS RATIO CA = <real>NUca_value
SHEAR MODULUS AB = <real>Gab_value
SHEAR MODULUS BC = <real>Gbc_value
SHEAR MODULUS CA = <real>Gca_value
COORDINATE SYSTEM = <string>coordinate_system_name
DIRECTION FOR ROTATION = <real>1|2|3
ALPHA = <real>alpha_in_degrees
SECOND DIRECTION FOR ROTATION = <real>1|2|3
SECOND ALPHA = <real>second_alpha_in_degrees
THERMAL STRAIN AA FUNCTION = <string>ethaa_function_name
THERMAL STRAIN BB FUNCTION = <string>ethbb_function_name
THERMAL STRAIN CC FUNCTION = <string>ethcc_function_name
END [PARAMETERS FOR MODEL ELASTIC_3D_ORTHOTROPIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Orthotropic crush

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
  <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
  <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
  <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL ORTHOTROPIC_CRUSH
YOUNGS MODULUS = <real>youngs_modulus
POISSONS RATIO = <real>poissons_ratio
SHEAR MODULUS = <real>shear_modulus
BULK MODULUS = <real>bulk_modulus
LAMBDA = <real>lambda
YIELD STRESS = <real>yield_stress
EX = <real>modulus_x
EY = <real>modulus_y
EZ = <real>modulus_z
GXY = <real>shear_modulus_xy
GYZ = <real>shear_modulus_yz
GZX = <real>shear_modulus_zx
VMIN = <real>min_crush_volume
CRUSH XX = <string>stress_volume_xx_function_name
CRUSH YY = <string>stress_volume_yy_function_name
CRUSH ZZ = <string>stress_volumezz_function_name
CRUSH XY = <string>shear_stress_volume_xy_function_name
CRUSH YZ = <string>shear_stress_volume_yz_function_name
CRUSH ZX = <string>shear_stress_volume_zx_function_name
END [PARAMETERS FOR MODEL ORTHOTROPIC_CRUSH]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Orthotropic rate

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
  DENSITY = <real>density_value
  #
  # {thermal strain option}
  THERMAL STRAIN FUNCTION = <string>thermal_strain_function
  # or all three of the following
  THERMAL STRAIN X FUNCTION = <string>thermal_strain_x_function
  THERMAL STRAIN Y FUNCTION = <string>thermal_strain_y_function
  THERMAL STRAIN Z FUNCTION = <string>thermal_strain_z_function
  #
  BEGIN PARAMETERS FOR MODEL ORTHOTROPIC_RATE
  YOUNGS MODULUS = <real>youngs_modulus
  POISSONS RATIO = <real>poissons_ratio
  SHEAR MODULUS = <real>shear_modulus
  BULK MODULUS = <real>bulk_modulus
  LAMBDA = <real>lambda
  YIELD STRESS = <real>yield_stress
  MODULUS TTTT = <real>modulus_tttt
  MODULUS TILL = <real>modulus_ttl1
  MODULUS TTWW = <real>modulus_ttww
  MODULUS LLLL = <real>modulus_llll
  MODULUS LLWW = <real>modulus_llww
  MODULUS WWWW = <real>modulus_wwww
  MODULUS TLTL = <real>modulus_tltl
  MODULUS LWLW = <real>modulus_lwlw
  MODULUS WTWT = <real>modulus_wttw
  TX = <real>tx
TY = <real>ty
TZ = <real>tz
LX = <real>lx
LY = <real>ly
LZ = <real>lz
MODULUS FUNCTION = <string>modulus_function_name
RATE FUNCTION = <string>rate_function_name
T FUNCTION = <string>t_function_name
L FUNCTION = <string>l_function_name
W FUNCTION = <string>w_function_name
TL FUNCTION = <string>tl_function_name
LW FUNCTION = <string>lw_function_name
WT FUNCTION = <string>wt_function_name
END [PARAMETERS FOR MODEL ORTHOTROPIC_RATE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Elastic laminate

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
BEGIN PARAMETERS FOR MODEL ELASTIC_LAMINATE
  A11 = <real>a11_value
  A12 = <real>a12_value
  A16 = <real>a16_value
  A22 = <real>a22_value
  A26 = <real>a26_value
  A66 = <real>a66_value
  A44 = <real>a44_value
  A45 = <real>a45_value
  A55 = <real>a55_value
  B11 = <real>b11_value
  B12 = <real>b12_value
  B16 = <real>b16_value
  B22 = <real>b22_value
  B26 = <real>b26_value
  B66 = <real>b66_value
  D11 = <real>d11_value
  D12 = <real>d12_value
  D16 = <real>d16_value
  D22 = <real>d22_value
  D26 = <real>d26_value
  D66 = <real>d66_value
COORDINATE SYSTEM = <string>coord_sys_name
DIRECTION FOR ROTATION = 1|2|3
ALPHA = <real>alpha_value_in_degrees
THETA = <real>theta_value_in_degrees
NTH11 FUNCTION = <string>nth11_function_name
NTH22 FUNCTION = <string>nth22_function_name
NTH12 FUNCTION = <string>nth12_function_name
MTH11 FUNCTION = <string>mth11_function_name
MTH22 FUNCTION = <string>mth22_function_name
MTH12 FUNCTION = <string>mth12_function_name
END [PARAMETERS FOR MODEL ELASTIC_LAMINATE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Fiber membrane

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
  <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
  <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
  <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL FIBER_MEMBRANE
  YOUNGS MODULUS = <real>youngs_modulus
  POISSONS RATIO = <real>poissons_ratio
  SHEAR MODULUS = <real>shear_modulus
  BULK MODULUS = <real>bulk_modulus
  LAMBDA = <real>lambda
  CORD DENSITY = <real>cord_density
  CORD DIAMETER = <real>cord_diameter
  MATRIX DENSITY = <real>matrix_density
  TENSILE TEST FUNCTION = <string>test_function_name
  PERCENT CONTINUUM = <real>percent_continuum
  EPL = <real>epl
  AXIS X = <real>axis_x
  AXIS Y = <real>axis_y
  AXIS Z = <real>axis_z
  MODEL = <string>RECTANGULAR
  STIFFNESS SCALE = <real>stiffness_scale
  REFERENCE STRAIN = <real>reference_strain
END [PARAMETERS FOR MODEL FIBER_MEMBRANE]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Incompressible solid

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
   <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
   <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
   <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL INCOMPRESSIBLE_SOLID
   YOUNGS MODULUS = <real>youngs_modulus
   POISSONS RATIO = <real>poissons_ratio
   BULK MODULUS = <real>bulk_modulus
   SHEAR MODULUS = <real>shear_modulus
   LAMBDA = <real>lambda
   K SCALING = <real>k_scaling
   2G SCALING = <real>2g_scaling
   TARGET E = <real>target_e
   MAX POISSONS RATIO = <real>max_poissons_ratio
   REFERENCE STRAIN = <real>reference_strain
   SCALING FUNCTION = <string>scaling_function_name
END [PARAMETERS FOR MODEL INCOMPRESSIBLE_SOLID]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]
#
# Mooney Rivlin

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
   DENSITY = <real>density_value
   #
BEGIN PARAMETERS FOR MODEL MOONEY_RIVLIN
   YOUNGS MODULUS = <real>youngs_modulus
   POISSONS RATIO = <real>poissons_ratio
   BULK MODULUS = <real>bulk_modulus
   SHEAR MODULUS = <real>shear_modulus
   LAMBDA = <real>lambda
   C10 = <real>c10
   C01 = <real>c01
   C10 FUNCTION = <string>c10_function_name
   C01 FUNCTION = <string>c01_function_name
   BULK FUNCTION = <string>bulk_function_name
   THERMAL EXPANSION FUNCTION = <string>eth_function_name
   TARGET E = <real>target_e
   TARGET E FUNCTION = <string>etar_function_name
   MAX POISSONS RATIO = <real>max_poissons_ratio
REFERENCE STRAIN = <real>reference_strain
END [PARAMETERS FOR MODEL MOONEY_RIVLIN]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# NVLE 3D Orthotropic

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
   DENSITY = <real>density_value
   #
   BEGIN PARAMETERS FOR MODEL NLVE_3D_ORTHOTROPIC
      YOUNGS MODULUS = <real>youngs_modulus
      POISSSONS RATIO = <real>poissons_ratio
      SHEAR MODULUS = <real>shear_modulus
      BULK MODULUS = <real>bulk_modulus
      LAMBDA = <real>lambda
      COORDINATE SYSTEM = <string>coordinate_system_name
      DIRECTION FOR ROTATION = <real>1|2|3
      ALPHA = <real>alpha_in_degrees
      SECOND DIRECTION FOR ROTATION = <real>1|2|3
      SECOND ALPHA = <real>second_alpha_in_degrees
      FICTITIOUS LOGA FUNCTION = <string>fict_loga_function_name
      FICTITIOUS LOGA SCALE FACTOR = <real>fict_loga_scale_factor
      # In each of the five ‘PRONY’ command lines and in
      # the RELAX TIME command line, the value of i can be from
      # 1 through 30
      1PSI PRONY <integer>i = <real>psi1_i
      2PSI PRONY <integer>i = <real>psi2_i
      3PSI PRONY <integer>i = <real>psi3_i
      4PSI PRONY <integer>i = <real>psi4_i
      5PSI PRONY <integer>i = <real>psi5_i
      RELAX TIME <integer>i = <real>tau_i
      REFERENCE TEMP = <real>tref
      REFERENCE DENSITY = <real>rhoref
      WLF C1 = <real>wlf_c1
      WLF C2 = <real>wlf_c2
      B SHIFT CONSTANT = <real>b_shift
      SHIFT REF VALUE = <real>shift_ref
      WWBETA 1PSI = <real>wwb_1psi
      WWTAU 1PSI = <real>wwt_1psi
      WWBETA 2PSI = <real>wwb_2psi
      WWTAU 2PSI = <real>wwt_2psi
      WWBETA 3PSI = <real>wwb_3psi
      WWTAU 3PSI = <real>wwt_3psi
      WWBETA 4PSI = <real>wwb_4psi
      WWTAU 4PSI = <real>wwt_4psi
      WWBETA 5PSI = <real>wwb_5psi
      WWTAU 5PSI = <real>wwt_5psi
DOUBLE INTEG FACTOR = \(<\text{real}>\text{dble\_int\_fac}\)

REF RUBBERY HCAPACITY = \(<\text{real}>\text{hcapr}\)

REF GLASSY HCAPACITY = \(<\text{real}>\text{hcapg}\)

GLASS TRANSITION TEM = \(<\text{real}>\text{tg}\)

REF GLASSY C11 = \(<\text{real}>\text{c11g}\)

REF RUBBERY C11 = \(<\text{real}>\text{c11r}\)

REF GLASSY C12 = \(<\text{real}>\text{c12g}\)

REF RUBBERY C12 = \(<\text{real}>\text{c12r}\)

REF GLASSY C13 = \(<\text{real}>\text{c13g}\)

REF RUBBERY C13 = \(<\text{real}>\text{c13r}\)

REF GLASSY C21 = \(<\text{real}>\text{c21g}\)

REF RUBBERY C21 = \(<\text{real}>\text{c21r}\)

REF GLASSY C22 = \(<\text{real}>\text{c22g}\)

REF RUBBERY C22 = \(<\text{real}>\text{c22r}\)

REF GLASSY C23 = \(<\text{real}>\text{c23g}\)

REF RUBBERY C23 = \(<\text{real}>\text{c23r}\)

REF GLASSY C31 = \(<\text{real}>\text{c31g}\)

REF RUBBERY C31 = \(<\text{real}>\text{c31r}\)

REF GLASSY C32 = \(<\text{real}>\text{c32g}\)

REF RUBBERY C32 = \(<\text{real}>\text{c32r}\)

REF GLASSY C33 = \(<\text{real}>\text{c33g}\)

REF RUBBERY C33 = \(<\text{real}>\text{c33r}\)

REF GLASSY C12 = \(<\text{real}>\text{c12g}\)

REF RUBBERY C12 = \(<\text{real}>\text{c12r}\)

REF GLASSY C13 = \(<\text{real}>\text{c13g}\)

REF RUBBERY C13 = \(<\text{real}>\text{c13r}\)

REF GLASSY C23 = \(<\text{real}>\text{c23g}\)

REF RUBBERY C23 = \(<\text{real}>\text{c23r}\)

REF GLASSY C44 = \(<\text{real}>\text{c44g}\)

REF RUBBERY C44 = \(<\text{real}>\text{c44r}\)

REF GLASSY C55 = \(<\text{real}>\text{c55g}\)

REF RUBBERY C55 = \(<\text{real}>\text{c55r}\)

REF GLASSY C66 = \(<\text{real}>\text{c66g}\)

REF RUBBERY C66 = \(<\text{real}>\text{c66r}\)

REF GLASSY CTE1 = \(<\text{real}>\text{cte1g}\)

REF RUBBERY CTE1 = \(<\text{real}>\text{cte1r}\)

REF GLASSY CTE2 = \(<\text{real}>\text{cte2g}\)

REF RUBBERY CTE2 = \(<\text{real}>\text{cte2r}\)

REF GLASSY CTE3 = \(<\text{real}>\text{cte3g}\)

REF RUBBERY CTE3 = \(<\text{real}>\text{cte3r}\)

LINEAR VISCO TEST = \(<\text{real}>\text{lvt}\)

T DERIV GLASSY C11 = \(<\text{real}>\text{dc11gdT}\)

T DERIV RUBBERY C11 = \(<\text{real}>\text{dc11rdT}\)

T DERIV GLASSY C22 = \(<\text{real}>\text{dc22gdT}\)

T DERIV RUBBERY C22 = \(<\text{real}>\text{dc22rdT}\)

T DERIV GLASSY C33 = \(<\text{real}>\text{dc33gdT}\)

T DERIV RUBBERY C33 = \(<\text{real}>\text{dc33rdT}\)

T DERIV GLASSY C12 = \(<\text{real}>\text{dc12gdT}\)

T DERIV RUBBERY C12 = \(<\text{real}>\text{dc12rdT}\)

T DERIV GLASSY C13 = \(<\text{real}>\text{dc13gdT}\)

T DERIV RUBBERY C13 = \(<\text{real}>\text{dc13rdT}\)

T DERIV GLASSY C23 = \(<\text{real}>\text{dc23gdT}\)

T DERIV RUBBERY C23 = \(<\text{real}>\text{dc23rdT}\)

T DERIV GLASSY C44 = \(<\text{real}>\text{dc44gdT}\)

T DERIV RUBBERY C44 = \(<\text{real}>\text{dc44rdT}\)

T DERIV GLASSY C55 = \(<\text{real}>\text{dc55gdT}\)

T DERIV RUBBERY C55 = \(<\text{real}>\text{dc55rdT}\)

T DERIV GLASSY C66 = \(<\text{real}>\text{dc66gdT}\)

T DERIV RUBBERY C66 = \(<\text{real}>\text{dc66rdT}\)
T DERIV GLASSY CTE1 = <real>dcte1gdT
T DERIV RUBBERY CTE1 = <real>dcte1rdT
T DERIV GLASSY CTE2 = <real>dcte2gdT
T DERIV RUBBERY CTE2 = <real>dcte2rdT
T DERIV GLASSY CTE3 = <real>dcte3gdT
T DERIV RUBBERY CTE3 = <real>dcte3rdT
T DERIV GLASSY HCAPACITY = <real>dhcapgdT
T DERIV RUBBERY HCAPACITY = <real>dhcaprdT
REF PSIC = <real>psic_ref
T DERIV PSIC = <real>dpsicdT
T 2DERIV PSIC = <real>d2psicdT2
PSI EQ 2T = <real>psitt
PSI EQ 3T = <real>psitttt
PSI EQ 4T = <real>psitttt
PSI EQ XX 11 = <real>psiXX11
PSI EQ XX 22 = <real>psiXX22
PSI EQ XX 33 = <real>psiXX33
PSI EQ XX 12 = <real>psiXX12
PSI EQ XX 13 = <real>psiXX13
PSI EQ XX 23 = <real>psiXX23
PSI EQ XX 44 = <real>psiXX44
PSI EQ XX 55 = <real>psiXX55
PSI EQ XX 66 = <real>psiXX66
PSI EQ XXT 11 = <real>psiXXT11
PSI EQ XXT 22 = <real>psiXXT22
PSI EQ XXT 33 = <real>psiXXT33
PSI EQ XXT 12 = <real>psiXXT12
PSI EQ XXT 13 = <real>psiXXT13
PSI EQ XXT 23 = <real>psiXXT23
PSI EQ XXT 44 = <real>psiXXT44
PSI EQ XXT 55 = <real>psiXXT55
PSI EQ XXT 66 = <real>psiXXT66
PSI EQ XT 1 = <real>psiXT1
PSI EQ XT 2 = <real>psiXT2
PSI EQ XT 3 = <real>psiXT3
PSI EQ XTT 1 = <real>psiXTT1
PSI EQ XTT 2 = <real>psiXTT2
PSI EQ XTT 3 = <real>psiXTT3
REF PSIA 11 = <real>psiA11
REF PSIA 22 = <real>psiA22
REF PSIA 33 = <real>psiA33
REF PSIA 12 = <real>psiA12
REF PSIA 13 = <real>psiA13
REF PSIA 23 = <real>psiA23
REF PSIA 44 = <real>psiA44
REF PSIA 55 = <real>psiA55
REF PSIA 66 = <real>psiA66
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T DERIV PSIA 11 = <real>dpsiA11dT
T DERIV PSIA 22 = <real>dpsiA22dT
T DERIV PSIA 33 = <real>dpsiA33dT
T DERIV PSIA 12 = <real>dpsiA12dT
T DERIV PSIA 13 = <real>dpsiA13dT
T DERIV PSIA 23 = <real>dpsiA23dT
T DERIV PSIA 44 = <real>dpsiA44dT
T DERIV PSIA 55 = <real>dpsiA55dT
T DERIV PSIA 66 = <real>dpsiA66dT
REF PSIB 1 = <real>psiB1
REF PSIB 2 = <real>psiB2
REF PSIB 3 = <real>psiB3
T DERIV PSIB 1 = <real>dpsiB1dT
T DERIV PSIB 2 = <real>dpsiB2dT
T DERIV PSIB 3 = <real>dpsiB3dT
PSI POT TT = <real>psipotTT
PSI POT TTT = <real>psipotTTT
PSI POT TTTT = <real>psipotTTTT
PSI POT XT 1 = <real>psipotXT1
PSI POT XT 2 = <real>psipotXT2
PSI POT XT 3 = <real>psipotXT3
PSI POT XT 11 = <real>psipotXT11
PSI POT XT 22 = <real>psipotXT22
PSI POT XT 33 = <real>psipotXT33
PSI POT XT 12 = <real>psipotXT12
PSI POT XT 13 = <real>psipotXT13
PSI POT XT 23 = <real>psipotXT23
PSI POT XT 44 = <real>psipotXT44
PSI POT XT 55 = <real>psipotXT55
PSI POT XT 66 = <real>psipotXT66
END [PARAMETERS FOR MODEL NLVE_3D_ORTHOTROPIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Stiff elastic

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value
#
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
  <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
<string>thermal_strain_z_function

# BEGIN PARAMETERS FOR MODEL STIFF_ELASTIC
YOUNGS MODULUS = <real>younsgs_modulus
POISSONS RATIO = <real>poissons_ratio
BULK MODULUS = <real>bulk_modulus
SHEAR MODULUS = <real>shear_modulus
LAMBDA = <real>lambda
SCALE FACTOR = <real>scale_factor
REFERENCE STRAIN = <real>reference_strain
END [PARAMETERS FOR MODEL STIFF_ELASTIC]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Swanson

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value

# BEGIN PARAMETERS FOR MODEL SWANSON
YOUNGS MODULUS = <real>younsgs_modulus
POISSONS RATIO = <real>poissons_ratio
BULK MODULUS = <real>bulk_modulus
SHEAR MODULUS = <real>shear_modulus
LAMBDA = <real>lambda
A1 = <real>a1
P1 = <real>p1
B1 = <real>b1
Q1 = <real>q1
C1 = <real>c1
R1 = <real>r1
CUT OFF STRAIN = <real>ecut
THERMAL EXPANSION FUNCTION = <string>eth_function_name
TARGET E = <real>target_e
TARGET E FUNCTION = <string>etar_function_name
MAX POISSONS RATIO = <real>max_poissons_ratio
REFERENCE STRAIN = <real>reference_strain
END [PARAMETERS FOR MODEL SWANSON]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Viscoelastic Swanson

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
DENSITY = <real>density_value

# BEGIN PARAMETERS FOR MODEL VISCOELASTIC_SWANSON
YOUNGS MODULUS = <real>younsgs_modulus
POISSONS RATIO = <real>poissons_ratio
BULK MODULUS = <real>bulk_modulus
SHEAR MODULUS = <real>shear_modulus
LAMBDA = <real>lambda
A1 = <real>a1
P1 = <real>p1
B1 = <real>b1
Q1 = <real>q1
C1 = <real>c1
R1 = <real>r1
CUT OFF STRAIN = <real>ecut
THERMAL EXPANSION FUNCTION = <string>eth_function_name
PRONY SHEAR INFINITY = <real>ginf
PRONY SHEAR 1 = <real>g1
PRONY SHEAR 2 = <real>g2
PRONY SHEAR 3 = <real>g3
PRONY SHEAR 4 = <real>g4
PRONY SHEAR 5 = <real>g5
PRONY SHEAR 6 = <real>g6
PRONY SHEAR 7 = <real>g7
PRONY SHEAR 8 = <real>g8
PRONY SHEAR 9 = <real>g9
PRONY SHEAR 10 = <real>g10
SHEAR RELAX TIME 1 = <real>tau1
SHEAR RELAX TIME 2 = <real>tau2
SHEAR RELAX TIME 3 = <real>tau3
SHEAR RELAX TIME 4 = <real>tau4
SHEAR RELAX TIME 5 = <real>tau5
SHEAR RELAX TIME 6 = <real>tau6
SHEAR RELAX TIME 7 = <real>tau7
SHEAR RELAX TIME 8 = <real>tau8
SHEAR RELAX TIME 9 = <real>tau9
SHEAR RELAX TIME 10 = <real>tau10
WLF COEF C1 = <real>wlf_c1
WLF COEF C2 = <real>wlf_c2
WLF TREF = <real>wlf_tref
NUMERICAL SHIFT FUNCTION = <string>ns_function_name
TARGET E = <real>target_e
TARGET E FUNCTION = <string>etar_function_name
MAX POISSONS RATIO = <real>max_poissons_ratio
REFERENCE STRAIN = <real>reference_strain
END [PARAMETERS FOR MODEL VISCOELASTIC_SWANSON]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Mie-Gruneisen

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL MIE_GRUNEISEN
    RHO_0 = <real>density
    C_0 = <real>sound_speed
    SHUG = <real>const_shock_velocity
    GAMMA_0 = <real>ambient_gruneisen_param
    POISSR = <real>poissons_ratio
    Y_0 = <real>yield_strength
    PMIN = <real>mean_stress(REAL_MAX)
END [PARAMETERS FOR MODEL MIE_GRUNEISEN]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Mie-Gruneisen power series

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
    <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
    <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
    <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL MIE_GRUNEISEN_POWER_SERIES
    RHO_0 = <real>density
    C_0 = <real>sound_speed
    K1 = <real>power_series_coeff1
    K2 = <real>power_series_coeff2
    K3 = <real>power_series_coeff3
    K4 = <real>power_series_coeff4
    K5 = <real>power_series_coeff5
    GAMMA_0 = <real>ambient_gruneisen_param
    POISSR = <real>poissons_ratio
    Y_0 = <real>yield_strength
    PMIN = <real>mean_stress(REAL_MAX)
END [PARAMETERS FOR MODEL MIE_GRUNEISEN_POWER_SERIES]
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END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# JWL (Jones-Wilkins-Lee)

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
  <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
  <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
  <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL JWL
  RHO_0 = <real>initial_density
  D = <real>detonation_velocity
  E_0 = <real>init_chem_energy
  A = <real>jwl_const_pressure1
  B = <real>jwl_const_pressure2
  R1 = <real>jwl_const_nondim1
  R2 = <real>jwl_const_nondim2
  OMEGA = <real>jwl_const_nondim3
  XDET = <real>x_detonation_point
  YDET = <real>y_detonation_point
  ZDET = <real>z_detonation_point
  TDET = <real>time_of_detonation
  B5 = <real>burn_width_const(2.5)
END [PARAMETERS FOR MODEL JWL]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Ideal gas

BEGIN PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name
# {thermal strain option}
THERMAL STRAIN FUNCTION = <string>thermal_strain_function
# or all three of the following
THERMAL STRAIN X FUNCTION =
  <string>thermal_strain_x_function
THERMAL STRAIN Y FUNCTION =
  <string>thermal_strain_y_function
THERMAL STRAIN Z FUNCTION =
  <string>thermal_strain_z_function
#
BEGIN PARAMETERS FOR MODEL IDEAL_GAS
  RHO_0 = <real>initial_density
C_0 = <real>initial_sound_speed
GAMMA = <real>ratio_specific_heats
END [PARAMETERS FOR MODEL IDEAL_GAS]
END [PROPERTY SPECIFICATION FOR MATERIAL <string>mat_name]

# Define mesh

BEGIN FINITE ELEMENT MODEL <string>mesh_descriptor
  DATABASE NAME = <string>mesh_file_name
  DATABASE TYPE = <string>database_type(exodusII)
  ALIAS <string>mesh_identifier AS <string>user_name
  OMIT BLOCK <string>block_list
  COMPONENT SEPARATOR CHARACTER = <string>separator
  BEGIN PARAMETERS FOR BLOCK <string list>block_names
    MATERIAL <string>material_name
    SOLID MECHANICS USE MODEL <string>model_name
    SECTION = <string>section_id
    LINEAR BULK VISCOSITY =
      <real>linear_bulk_viscosity_value(0.06)
    QUADRATIC BULK VISCOSITY =
      <real>quad_bulk_viscosity_value(1.20)
    HOURGLASS STIFFNESS =
      <real>hour_glass_stiff_value(solid = 0.05, shell/membrane = 0.0)
    HOURGLASS VISCOSITY =
      <real>hour_glass_visc_value(solid = 0.0, shell/membrane = 0.0)
    EFFECTIVE MODULI MODEL = <string>PRESTO|PRONTO|
      CURRENT|ELASTIC(PRONTO)
    ELEMENT NUMERICAL FORMULATION = <string>OLD|NEW(OLD)
    ACTIVE FOR PROCEDURE <string>proc_name DURING PERIODS
    <string list>period_names
  END [PARAMETERS FOR BLOCK <string list>block_names]
END [FINITE ELEMENT MODEL <string>mesh_descriptor]

# Element sections

BEGIN SOLID SECTION <string>solid_section_name
  FORMULATION = <string>MEAN_QUADRATURE|
    SELECTIVE_DEVIATORIC(MEAN QUADRATURE)
  DEVIATORIC PARAMETER = <real>deviatoric_param
  STRAIN INCREMENTATION = <string>MIDPOINT_INCREMENT|
    STRONGLY_OBJECTIVE|NODE_BASED(MIDPOINT_INCREMENT)
  NODE BASED ALPHA FACTOR =
    <real>bulk_stress_weight(0.01)
  NODE BASED BETA FACTOR =
    <real>shear stress_weight(0.35)
RIGID BODY = <string>rigid_body_name
END [SOLID SECTION <string>solid_section_name]

BEGIN SHELL SECTION <string>shell_section_name
THICKNESS = <real>shell_thickness
THICKNESS MESH VARIABLE =
   <string>THICKNESS|<string>var_name
THICKNESS TIME STEP = <real>time_value
THICKNESS SCALE FACTOR = <real>thick_scale_factor(1.0)
INTEGRATION RULE = TRAPEZOID|GAUSS|LOBATTO|SIMPSONS|
   USER(TRAPEZOID)
NUMBER OF INTEGRATION POINTS =
   <integer>num_int_points(5)
BEGIN USER INTEGRATION RULE
   <real>location_1 <real>weight_1
   <real>location_2 <real>weight_2
   .
   .
   <real>location_n <real>weight_n
END [USER INTEGRATION RULE]
LOFTING FACTOR = <real>lofting_factor(0.5)
ORIENTATION = <string>orientation_name
RIGID BODY = <string>rigid_body_name
END [SHELL SECTION <string>shell_section_name]

BEGIN MEMBRANE SECTION <string>membrane_section_name
THICKNESS = <real>mem_thickness
THICKNESS MESH VARIABLE =
   <string>THICKNESS|<string>var_name
THICKNESS TIME STEP = <real>time_value
THICKNESS SCALE FACTOR = <real>thick_scale_factor(1.0)
FORMULATION = <string>MEAN_QUADRATURE|
   SELECTIVE_DEVIATORIC(MEAN QUADRATURE)
DEVIATORIC PARAMETER = <real>deviatoric_param
LOFTING FACTOR = <real>lofting_factor(0.5)
RIGID BODY = <string>rigid_body_name
END [MEMBRANE SECTION <string>membrane_section_name]

BEGIN BEAM SECTION <string>beam_section_name
SECTION = <string>ROD|TUBE|BAR|BOX|I
WIDTH = <real>section_width
HEIGHT = <real>section_width
WALL THICKNESS = <real>wall_thickness
FLANGE THICKNESS = <real>flange_thickness
T AXIS = <real>tx <real>ty <real>tz (0 0 1)
REFERENCE AXIS = <string>CENTER|RIGHT|
   TOP|LEFT|BOTTOM (CENTER)
AXIS OFFSET = <real>s_offset <real>t_offset
RIGID BODY = <string>rigid_body_name
END [BEAM SECTION <string>beam_section_name]

BEGIN TRUSS SECTION <string>truss_section_name
  AREA = <real>cross_sectional_area
  INITIAL LOAD = <real>initial_load
  PERIOD = <real>period
  RIGID BODY = <string>rigid_body_name
END [TRUSS SECTION <string>truss_section_name]

BEGIN DAMPER SECTION <string>damper_section_name
  AREA = <real>damper_cross_sectional_area
END [DAMPER SECTION <string>damper_section_name]

BEGIN POINT MASS SECTION <string>pointmass_section_name
  VOLUME = <real>volume
  RIGID BODY = <string>rigid_body_name
END [POINT MASS SECTION <string>pointmass_section_name]

BEGIN SPH SECTION <string>sph_section_name
  RADIUS MESH VARIABLE =
    <string>var_name|<string>attribute|SPHERE INITIAL
  RADIUS = <real>rad
  RADIUS MESH VARIABLE TIME STEP = <string>time
  PROBLEM DIMENSION = <integer>1|2|3(3)
  CONSTANT SPHERE RADIUS
END [SPH SECTION <string>sph_section_name]

# SPH utility commands
SPH SYMMETRY PLANE <string>+X|+Y|+Z|-X|-Y|-Z
<real>position_on_axis(0.0)
SPH DECOUPLE STRAINS: <string>material1 <string>material2

# Zoltan parameters
BEGIN ZOLTAN PARAMETERS <string>parameter_name
  LOAD BALANCING METHOD = <string>recursive coordinate
    bisection|recursive inertial bisection|hilbert space
    filling curve|octree
  DETERMINISTIC DECOMPOSITION = <string>false|true
  IMBALANCE TOLERANCE = <real>imb_tol
  OVER_ALLOCATE MEMORY = <real>over_all_mem
  REUSE CUTS = <string>false|true
  ALGORITHM DEBUG LEVEL = <integer>alg_level
    # 0<=(alg_level)<=3
CHECK GEOMETRY = <string>false|true
KEEP CUTS = <string>false|true
LOCK RCB DIRECTIONS = <string>false|true
SET RCB DIRECTIONS = <string>do not order cuts|xyz|xzy|yzx|yxz|zxy|zyx
RECTILINEAR RCB BLOCKS = <string>false|true
RENUMBER PARTITIONS = <string>false|true
OCTREE DIMENSION = <integer>oct_dimension
OCTREE METHOD = <string>morton indexing|grey code|hilbert
OCTREE MIN OBJECTS = <integer>min_obj # 1<= (min_obj)
OCTREE MAX OBJECTS = <integer>max_obj # 1<= (max_obj)
ZOLTAN DEBUG LEVEL = <integer>zoltan_level
    # 0<=(zoltan_level)<=10
DEBUG PROCESSOR NUMBER = <integer>proc # 1<=proc
TIMER = <string>wall|cpu
DEBUG MEMORY = <integer>dbg_mem # 0<=(dbg_mem)<=3
END [ZOLTAN PARAMETERS <string>parameter_name]

# Output scheduler
BEGIN OUTPUT SCHEDULER <string>scheduler_name
START TIME = <real>output_start_time
TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
AT TIME <real>time_begin INCREMENT =
    <real>time_increment_dt
ADDITIONAL TIMES = <real>output_time1
    <real>output_time2 ...
AT STEP <integer>step_begin INCREMENT =
    <integer>step_increment
ADDITIONAL STEPS = <integer>output_step1
    <integer>output_step2 ...
TERMINATION TIME = <real>termination_time_value
END [OUTPUT SCHEDULER <string>scheduler_name]

# Begin Procedure scope
BEGIN PRESTO PROCEDURE <string>presto_procedure_name

# Time block
BEGIN TIME CONTROL
BEGIN TIME STEPPING BLOCK <string>time_block_name
START TIME = <real>start_time_value
BEGIN PARAMETERS FOR PRESTO REGION
    <string>region_name
    INITIAL TIME STEP = <real>initial_time_step_value
    TIME STEP SCALE FACTOR =
TIME STEP INCREASE FACTOR =
<real>time_step_increase_factor(1.1)
STEP INTERVAL = <integer>nsteps(100)
END [PARAMETERS FOR PRESTO REGION
<string>region_name]
END [TIME STEPPING BLOCK <string>time_block_name]
TERMINATION TIME = <real>termination_time
END TIME CONTROL

# Begin Region scope

BEGIN PRESTO REGION <string>presto_region_name

USE FINITE ELEMENT MODEL <string>model_name

# Error controller

USE ERROR ESTIMATION CONTROLLER <string>err_name

# Time step control using Lanczos

BEGIN LANCZOS PARAMETERS <string>lanczos_name
    NUMBER EIGENVALUES = <integer>num_eig(20)
    STARTING VECTOR = <string>STRETCH_X|STRETCH_Y|STRETCH_Z
      (STRETCH_X)
    VECTOR SCALE = <real>vec_scale(1.0e-5)
    TIME SCALE = <real>time_scale(0.9)
    STEP INTERVAL = <integer>step_int(500)
    INCREMENT INTERVAL = <integer>incr_int(5)
    TIME STEP LIMIT = <real>step_lim(0.10)
END [LANCZOS PARAMETERS <string>lanczos_name]

# Time step control using nodes

BEGIN NODE BASED TIME STEP PARAMETERS <string>nbased_name
    INCREMENT INTERVAL = <integer>incr_int(5)
    STEP INTERVAL = <integer>step_int(500)
    TIME STEP LIMIT = <real>step_lim(0.10)
END [NODE BASED TIME STEP PARAMETERS <string>nbased_name]

# Mass scaling

BEGIN MASS SCALING
  # (node set commands)
  NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names

#
TARGET TIME STEP = <real>target_time_step
ALLOWABLE MASS INCREASE RATIO
  = <real>mass_increase_ratio
#
# additional command
ACTIVE PERIODS = <string list>periods
END MASS SCALING

# Energy deposition

BEGIN PRESCRIBED ENERGY DEPOSITION
  # {block set commands}
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE BLOCK
  #
  # function commands
  T FUNCTION = <string>t_func_name
  X FUNCTION = <string>x_func_name
  Y FUNCTION = <string>y_func_name
  Z FUNCTION = <string>z_func_name
  #
  # input mesh command
  READ VARIABLE = <string>mesh_var_name
  #
  # user subroutine commands
  ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value
END [PRESCRIBED ENERGY DEPOSITION]

# Torsional spring

BEGIN TORSIONAL SPRING MECHANISM <string>spring_name
  NODE SETS = <string>nodelist_int1
BEGIN MASS PROPERTIES
# {block set commands}
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE BLOCK = <string list>block_names
#
# structure command
STRUCTURE NAME = <string>structure_name
END [MASS PROPERTIES]

BEGIN ELEMENT DEATH <string>death_name
# {block set commands}
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE BLOCK = <string list>block_names
#
# criteria commands
CRITERION IS AVG|MAX|MIN NODAL VALUE OF
   <string>var_name[(<integer>component_num)]
   |<|<=|=|>=|>| <real>tolerance
CRITERION IS ELEMENT VALUE OF
   <string>var_name[(<integer>component_num)]
   |<|<=|=|>=|>| <real>tolerance |
   <string>derived_quantity[(<integer>component_num)]
   |<|<=|=|>=|>| <real>tolerance
CRITERION IS GLOBAL VALUE OF
   <string>var_name[(<integer>component_num)]
   |<|<=|=|>=|>| <real>tolerance
ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
   = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
   = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
= <string>param_value
MATERIAL CRITERION
  = <string list>material_model_names

# evaluation commands
CHECK STEP INTERVAL = <integer>num_steps
CHECK TIME INTERVAL = <real>delta_t
DEATH START TIME = <real>time

# miscellaneous option commands
DEATH STEPS = <integer>death_steps(1)
FORCE VALID ACME CONNECTIVITY

# additional command
ACTIVE PERIODS = <string list>period_names
END [ELEMENT DEATH <string>death_name]

# Derived output
BEGIN DERIVED OUTPUT
  COMPUTE AND STORE STRESS VARIABLE =<string>derived_quantity_name
END DERIVED OUTPUT

# Mesh rebalance
BEGIN REBALANCE
  INITIAL REBALANCE = ON|OFF(OFF)
  PERIODIC REBALANCE = ON|OFF|AUTO(OFF)
  STEP INTERVAL = <integer>step_interval
  COMMUNICATION RATIO THRESHOLD = <real>ratio
  ZOLTAN PARAMETERS = <string>parameter_name
END REBALANCE

# Initial condition
BEGIN INITIAL CONDITION
# (mesh-entity set commands)
NODE_SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE_SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
#
# variable identification commands
INITIALIZE VARIABLE NAME = <string>var_name
VARIABLE TYPE = [NODE|EDGE|FACE|ELEMENT|GLOBAL]
#
# constant magnitude command
MAGNITUDE = <real list>initial_values
#
# input mesh commands
READ VARIABLE = <string>mesh_var_name
TIME = <real>time
#
# user subroutine commands
NODE_SET_SUBROUTINE = <string>subroutine_name |
SURFACE_SUBROUTINE = <string>subroutine_name |
ELEMENT_BLOCK_SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
   = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
   = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
   = <string>param_value
#
# additional command
SCALE FACTOR = <real>scale_factor(1.0)
END [INITIAL CONDITION]

# Boundary conditions
BEGIN FIXED DISPLACEMENT
# (node set commands)
NODE_SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE_SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
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# component commands
COMPONENT = <string>X/Y/Z | COMPONENTS =
  <string>X/Y/Z
#
# additional command
ACTIVE PERIODS = <string list>period_names
END [FIXED DISPLACEMENT]

BEGIN PRESCRIBED DISPLACEMENT
  # {node set commands}
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names
#
# function commands
  DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z |
    CYLINDRICAL AXIS = <string>defined_axis |
    RADIAL AXIS = <string>defined_axis
  FUNCTION = <string>function_name
#
# user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
  SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
  SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
#
# additional commands
  SCALE FACTOR = <real>scale_factor(1.0)
  ACTIVE PERIODS = <string list>period_names
END [PRESCRIBED DISPLACEMENT]

BEGIN PRESCRIBED VELOCITY
  # {node set commands}
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
#
# function commands
DIRECTION = <string>defined_direction | COMPONENT = <string>X|Y|Z |
CYLINDRICAL AXIS = <string>defined_axis |
RADIAL AXIS = <string>defined_axis
FUNCTION = <string>function_name
#
# user subroutine commands
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
= <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
= <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
= <string>param_value
#
# additional commands
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
END [PRESCRIBED VELOCITY]

BEGIN PRESCRIBED ACCELERATION
# (node set commands)
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
#
# function commands
DIRECTION = <string>defined_direction | COMPONENT = <string>X|Y|Z
FUNCTION = <string>function_name
#
# user subroutine commands
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
= <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
= <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
= <string>param_value
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SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value

# additional commands
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names

BEGIN FIXED ROTATION
  # {node set commands}
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names

  # component commands
  COMPONENT = <string>X/Y/Z | COMPONENTS =
    <string>X/Y/Z

  # additional command
  ACTIVE PERIODS = <string list>periods_names

END [FIXED ROTATION]

BEGIN PRESCRIBED ROTATION
  # {node set commands}
  NODE SET = <string list>nodelist_names
  SURFACE = <string list>surface_names
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE NODE SET = <string list>nodelist_names
  REMOVE SURFACE = <string list>surface_names
  REMOVE BLOCK = <string list>block_names

  # function commands
  DIRECTION = <string>defined_direction | COMPONENT = <string>X|Y|Z
  FUNCTION = <string>function_name

  # user subroutine commands
  NODE SET SUBROUTINE = <string>subroutine_name
  SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
  SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name = <string>param_value
#
# additional commands
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
END [PRESCRIBED ROTATION]

BEGIN INITIAL VELOCITY
# (node set commands)
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
#
# direction commands
COMPONENT = <string>X|Y|Z |
   DIRECTION = <string>defined_direction
MAGNITUDE = <real>magnitude_of_velocity
#
# angular velocity commands
# CYLINDRICAL AXIS = <string>defined_axis
ANGULAR VELOCITY = <real>angular_velocity
#
# user subroutine commands
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name = <string>param_value
END [INITIAL VELOCITY]

BEGIN PRESSURE
# (surface set commands)
SURFACE = <string list>surface_names
REMOVE SURFACE = <string list>surface_names
#
# function command
FUNCTION = <string>function_name
# user subroutine commands
SURFACE SUBROUTINE = <string>subroutine_name
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value

# external pressure sources
READ VARIABLE = <string>variable_name
OBJECT TYPE = <string>NODE|FACE(NODE)
TIME = <real>time
FIELD VARIABLE = <string>field_variable

# output external forces from pressure
EXTERNAL FORCE CONTRIBUTION OUTPUT NAME
  = <string>variable_name

# additional commands
USE DEATH = <string>death_name
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names

END [PRESSURE]

BEGIN TRACTION
  # {surface set commands}
SURFACE = <string list>surface_names
REMOVE SURFACE = <string list>surface_names

  # function commands
DIRECTION = <string>direction_name
FUNCTION = <string>function_name

  # user subroutine commands
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
  = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
  = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
  = <string>param_value

#
# additional commands
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
END [TRACTION]

BEGIN PRESCRIBED FORCE
# {node set commands}
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
#
# function commands
DIRECTION = <string>defined_direction |
    COMPONENT = <string>X|Y|Z
FUNCTION = <string>function_name
#
# user subroutine commands
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
    = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
#
# additional commands
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
END [PRESCRIBED FORCE]

BEGIN PRESCRIBED MOMENT
# {node set commands}
NODE SET = <string list>nodelist_names
SURFACE = <string list>surface_names
BLOCK = <string list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list>surface_names
REMOVE BLOCK = <string list>block_names
#
# function commands
DIRECTION = <string>defined_direction |
COMPONENT = <string>X|Y|Z
FUNCTION = <string>function_name
#
# user subroutine commands
NODE SET SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
   = <real>param_value
SUBROUTINE INTEGER PARAMETER: <string>param_name
   = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
   = <string>param_value
#
# additional commands
SCALE FACTOR = <real>scale_factor(1.0)
ACTIVE PERIODS = <string list>period_names
END [PRESCRIBED MOMENT]

# Standard temperature boundary condition

BEGIN PRESCRIBED TEMPERATURE
   # {block set commands}
   BLOCK = <string_list>block_names
   INCLUDE ALL BLOCKS
   REMOVE BLOCK
   #
   # function command
   FUNCTION = <string>function_name
   #
   # user subroutine commands
   NODE SET SUBROUTINE = <string>subroutine_name
   SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
   SUBROUTINE REAL PARAMETER: <string>param_name
      = <real>param_value
   SUBROUTINE INTEGER PARAMETER: <string>param_name
      = <integer>param_value
   SUBROUTINE STRING PARAMETER: <string>param_name
      = <string>param_value
   #
   # read variable commands
   READ VARIABLE = <string>variable_name
   TIME = <real>time
   #
   # additional commands
   SCALE FACTOR = <real>scale_factor(1.0)
   ACTIVE PERIODS = <string list>period_names
END [PRESCRIBED TEMPERATURE]
# Specialized boundary conditions

BEGIN GRAVITY
   # {node set commands}
   NODE SET = <string list>nodelist_names
   SURFACE = <string list>surface_names
   BLOCK = <string list>block_names
   INCLUDE ALL BLOCKS
   REMOVE NODE SET = <string list>nodelist_names
   REMOVE SURFACE = <string list>surface_names
   REMOVE BLOCK = <string list>block_names
   #
   DIRECTION = <string>defined_direction
   FUNCTION = <string>function_name
   GRAVITATIONAL CONSTANT = <real>g_constant
   SCALE FACTOR = <real>scale_factor(1.0)
   ACTIVE PERIODS = <string list>period_names
END [GRAVITY]

BEGIN CAVITY EXPANSION
   EXPANSION RADIUS = <string>SPHERICAL|CYLINDRICAL
   (spherical)
   SURFACE = <string list>surface_ids
   REMOVE SURFACE = <string list>surface_ids
   FREE SURFACE = <real>top_surface_zcoord
                  <real>bottom_surface_zcoord
   NODE SETS TO DEFINE BODY AXIS = <string>nodelist_1 <string>nodelist_id2
   TIP RADIUS = <real>tip_radius
   BEGIN LAYER <string>layer_name
      LAYER SURFACE = <real>top_layer_zcoord
                      <real>bottom_layer_zcoord
      PRESSURE COEFFICIENTS = <real>c0 <real>c1
                              <real>c2
      SURFACE EFFECT = <string>NONE|SIMPLE_ON_OFF(NONE)
      FREE SURFACE EFFECT COEFFICIENTS = <real>coeff1
                                          <real>coeff2
   END [LAYER <string>layer_name]
   ACTIVE PERIODS = <string list>period_names
END [CAVITY EXPANSION]

BEGIN SILENT BOUNDARY
   SURFACE = <string list>surface_names
   REMOVE SURFACE = <string list>surface_names
   ACTIVE PERIODS = <string list>period_names
END [SILENT BOUNDARY]
BEGIN SPOT WELD
  NODE SET = <string list>nodelist_ids
  REMOVE NODE SET = <string list>nodelist_ids
  SURFACE = <string list>surface_ids
  REMOVE SURFACE = <string list>surfac_ids
  SECOND SURFACE = <string>surface_id
  NORMAL DISPLACEMENT FUNCTION =
    <string>function_nor_disp
  NORMAL DISPLACEMENT SCALE FACTOR =
    <real>scale_nor_disp[1.0]
  TANGENTIAL DISPLACEMENT FUNCTION =
    <string>function_tang_disp
  TANGENTIAL DISPLACEMENT SCALE FACTOR =
    <real>scale_tang_disp[1.0]
  FAILURE ENVELOPE EXPONENT = <real>exponent
  FAILURE FUNCTION = <string>fail_func_name
  FAILURE DECAY CYCLES = <integer>number_decay_cycles
  SEARCH TOLERANCE = <real>search_tolerance
  IGNORE INITIAL OFFSET = NO|YES[NO]
  ACTIVE PERIODS = <string list>period_names
END [SPOT WELD]

BEGIN LINE WELD
  SURFACE = <string list> surface_names
  REMOVE SURFACE = <string list> surface_names
  BLOCK = <string list> block_names
  REMOVE BLOCK = <string list>block_names
  SEARCH TOLERANCE = <real>search_tolerance
  R DISPLACEMENT FUNCTION =
    <string>r_disp_function_name
  R DISPLACEMENT SCALE FACTOR = <real>r_disp_scale
  S DISPLACEMENT FUNCTION =
    <string>s_disp_function_name
  S DISPLACEMENT SCALE FACTOR = <real>s_disp_scale
  T DISPLACEMENT FUNCTION =
    <string>t_disp_function_name
  T DISPLACEMENT SCALE FACTOR = <real>t_disp_scale
  R ROTATION FUNCTION =
    <string>r_rotation_function_name
  R ROTATION SCALE FACTOR = <real>r_rotation_scale
  S ROTATION FUNCTION =
    <string>s_rotation_function_name
  S ROTATION SCALE FACTOR = <real>s_rotation_scale
  T ROTATION FUNCTION =
    <string>t_rotation_function_name
  T ROTATION SCALE FACTOR = <real>t_rotation_scale
FAILURE ENVELOPE EXPONENT = <real>k
FAILURE DECAY CYCLES = <integer>number_decay_cycles
ACTIVE PERIODS = <string list>period_names
END [LINE WELD]

BEGIN VISCOUS DAMPING <string>damp_name
  # {block set commands}
  BLOCK = <string list>block_names
  INCLUDE ALL BLOCKS
  REMOVE BLOCK = <string list>block_names
  #
  MASS DAMPING COEFFICIENT = <real>mass_damping
  STIFFNESS DAMPING COEFFICIENT = <real>stiff_damping
  #
  # additional command
  ACTIVE PERIODS = <string list>period_names
END [VISCOUS DAMPING <string>damp_name]

# Contact

BEGIN CONTACT DEFINITION <string>name
  #
  # contact surface and node set definition
  CONTACT SURFACE <string>name
    CONTAINS <string list>surface_names
    #
    SKIN ALL BLOCKS = <string>ON|OFF(OFF)
      [EXCEPT <string list> block_names]
    #
  BEGIN CONTACT SURFACE <string>name
    BLOCK = <string list>block_names
    SURFACE = <string list>surface_names
    NODE SET = <string list>node_set_names
    REMOVE BLOCK = <string list>block_names
    REMOVE SURFACE = <string list>surface_names
    REMOVE NODE SET = <string list>nodelist_names
  END [CONTACT SURFACE <string>name]
  #
  CONTACT NODE SET <string>surface_name
    CONTAINS <string>nodelist_names
    #
    # analytic surfaces
  BEGIN ANALYTIC PLANE <string>name
    NORMAL = <string>defined_direction
    POINT = <string>defined_point
  END [ANALYTIC PLANE <string>name]
  #
BEGIN ANALYTIC CYLINDER <string>name
    CENTER = <string>defined_point
    AXIAL DIRECTION = <string>defined_axis
    RADIUS = <real>cylinder_radius
    LENGTH = <real>cylinder_length
    CONTACT NORMAL = <string>OUTSIDE|INSIDE
END [ANALYTIC CYLINDER <string>name]
#
BEGIN ANALYTIC SPHERE <string>name
    CENTER = <string>defined_point
    RADIUS = <real>sphere_radius
END [ANALYTIC SPHERE <string>name]
# end contact surface and node set definition
#
UPDATE ALL SURFACES FOR ELEMENT DEATH = <string>ON|OFF(ON)
#
BEGIN REMOVE INITIAL OVERLAP
    OVERLAP NORMAL TOLERANCE = <real>over_norm_tol
    OVERLAP TANGENTIAL TOLERANCE = <real>over_tang_tol
    SHELL OVERLAP ITERATIONS = <integer>max_iter(10)
    SHELL OVERLAP TOLERANCE = <real>shell_over_tol(0.0)
END [REMOVE INITIAL OVERLAP]
#
MULTIPLE INTERACTIONS = <string>ON|OFF(ON)
MULTIPLE INTERACTIONS WITH ANGLE = <real>angle(60.0)
#
SURFACE NORMAL SMOOTHING = <string>ON|OFF(OFF)
#
ERODED FACE TREATMENT = <string>NONE|ALL(ALL)
#
# shell lofting
BEGIN SHELL LOFTING
    LOFTING ALGORITHM = <string>ON|OFF(ON)
    COINCIDENT SHELL TREATMENT = <string>DISALLOW|IGNORE|SIMPLE(DISALLOW)
    COINCIDENT SHELL HEX TREATMENT = <string>DISALLOW|IGNORE|TAPERED|EMBEDDED(DISALLOW)
END [SHELL LOFTING]
# end shell lofting
#
# surface-physics models
BEGIN FRICTIONLESS MODEL <string>name
END [FRICTIONLESS MODEL <string>name]
#
BEGIN CONSTANT FRICTION MODEL <string>name
    FRICTION COEFFICIENT = <real>coeff
END [CONSTANT FRICTION MODEL <string>name]
# BEGIN TIED MODEL <string>name
END [TIED MODEL <string>name]
#
BEGIN SPRING WELD MODEL <string>name
   NORMAL DISPLACEMENT FUNCTION = <string>func_name
   NORMAL DISPLACEMENT SCALE FACTOR = <real>scale_factor(1.0)
   TANGENTIAL DISPLACEMENT FUNCTION = <string>func_name
   TANGENTIAL DISPLACEMENT SCALE FACTOR = <real>scale_factor(1.0)
   FAILURE ENVELOPE EXPONENT = <real>exponent(2.0)
   FAILURE DECAY CYCLES = <integer>num_cycles(1)
   FAILED MODEL = <string>failed_model_name|FRICTIONLESS (FRICTIONLESS)
END [SPRING WELD MODEL <string>name]
#
BEGIN SURFACE WELD MODEL <string>name
   NORMAL CAPACITY = <real>normal_cap
   TANGENTIAL CAPACITY = <real>tangential_cap
   FAILURE DECAY CYCLES = <integer>num_cycles(1)
   FAILED MODEL = <string>failed_model_name|FRICTIONLESS (FRICTIONLESS)
END [SURFACE WELD MODEL <string>name]
#
BEGIN AREA WELD MODEL <string>name
   NORMAL CAPACITY = <real>normal_cap
   TANGENTIAL CAPACITY = <real>tangential_cap
   FAILURE DECAY CYCLES = <integer>num_cycles(1)
   FAILED MODEL = <string>failed_model_name|FRICTIONLESS (FRICTIONLESS)
END [AREA WELD MODEL <string>name]
#
BEGIN ADHESION MODEL <string>name
   ADHESION FUNCTION = <string>func_name
   ADHESION SCALE FACTOR = <real>scale_factor(1.0)
END [ADHESION MODEL <string>name]
#
BEGIN COHESIVE ZONE MODEL <string>name
   TRACTION DISPLACEMENT FUNCTION = <string>func_name
   TRACTION DISPLACEMENT SCALE FACTOR = <real>scale_factor(1.0)
   CRITICAL NORMAL GAP = <real>crit_norm_gap
   CRITICAL TANGENTIAL GAP = <real>crit_tangential_gap
END [COHESIVE ZONE MODEL <string>name]
#
BEGIN JUNCTION MODEL <string>name
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NORMAL TRACTION FUNCTION = <string>func_name
NORMAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
TANGENTIAL TRACTION FUNCTION = <string>func_name
TANGENTIAL TRACTION SCALE FACTOR =
   <real>scale_factor(1.0)
NORMAL CUTTOFF DISTANCE FOR TANGENTIAL TRACTION =
   <real>distance
END [JUNCTION MODEL <string>name]
#
BEGIN THREADED MODEL <string>name
NORMAL TRACTION FUNCTION = <string>func_name
NORMAL TRACTION SCALE FACTOR = <real>scale_factor(1.0)
TANGENTIAL TRACTION FUNCTION = <string>func_name
TANGENTIAL TRACTION SCALE FACTOR =
   <real>scale_factor(1.0)
TANGENTIAL TRACTION GAP FUNCTION = <string>func_name
TANGENTIAL TRACTION GAP SCALE FACTOR =
   <real>scale_factor(1.0)
NORMAL CAPACITY = <real>normal_cap
TANGENTIAL CAPACITY = <real>tangential_cap
FAILURE ENVELOPE EXponent = <real>exponent(2.0)
FAILURE DECAY CYCLES = <integer>num_cycles(1)
FAILED MODEL = <string>failed_model_name|FRICTIONLESS
   (FRICTIONLESS)
END [THREADED MODEL <string>name]
#
BEGIN PV_DEPENDENT MODEL <string>name
   STATIC COEFFICIENT = <real>stat_coeff
   DYNAMIC COEFFICIENT = <real>dyn_coeff
   VELOCITY DECAY = <real>vel_decay
   REFERENCE PRESSURE = <real>p_ref
   OFFSET PRESSURE = <real>p_off
   PRESSURE EXPONENT = <real>p_exp
END [PV_DEPENDENT MODEL <string>name]
# end surface physics models
#
BEGIN USER SUBROUTINE MODEL <string>name
   INITIALIZE MODEL SUBROUTINE = <string>init_model_name
   INITIALIZE TIME STEP SUBROUTINE = <string>init_ts_name
   INITIALIZE NODE STATE DATA SUBROUTINE =
     <string>init_node_data_name
   LIMIT FORCE SUBROUTINE = <string>limit_force_name
   ACTIVE SUBROUTINE = <string>active_name
   INTERACTION TYPE SUBROUTINE = <string>interaction_name
END [USER SUBROUTINE MODEL <string>name]
#
# search options command block
BEGIN SEARCH OPTIONS [<string>name]
  GLOBAL SEARCH INCREMENT = <integer>num_steps(1)
  GLOBAL SEARCH ONCE = <string>ON|OFF(OFF)
  SEARCH TOLERANCE = <string>AUTOMATIC|USER_DEFINED
    (AUTOMATIC)
  NORMAL TOLERANCE = <real>norm_tol
  TANGENTIAL TOLERANCE = <real>tang_tol
  SECONDARY DECOMPOSITION = <string>ON|OFF(ON)
END [SEARCH OPTIONS <string>name]

# enforcement
BEGIN ENFORCEMENT OPTIONS [<string>name]
  ENFORCEMENT ALGORITHM = <string>MOMENTUM_BALANCE|
    PENALTY(MOMENTUM_BALANCE)
  MOMENTUM BALANCE ITERATIONS = <integer>num_iter(5)
END [ENFORCEMENT OPTIONS <string>name]

# BEGIN INTERACTION DEFAULTS [<string>name]
  SURFACES = <string list>surface_names
  SELF CONTACT = <string>ON|OFF(OFF)
  GENERAL CONTACT = <string>ON|OFF(OFF)
  AUTOMATIC KINEMATIC PARTITION = <string>ON|OFF(OFF)
  INTERACTION BEHAVIOR = <string>SLIDING|
    INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)
  FRICTION MODEL = <string>friction_model_name|
    FRICTIONLESS(FRICTIONLESS)
END [INTERACTION DEFAULTS <string>name]

# BEGIN INTERACTION [<string>name]
  SURFACES = <string>surface1 <string>surface2
  MASTER = <string>surface
  SLAVE = <string>surface
  KINEMATIC PARTITION = <real>kin_part
  NORMAL TOLERANCE = <real>norm_tol
  TANGENTIAL TOLERANCE = <real>tang_tol
  OVERLAP NORMAL TOLERANCE = <real>over_norm_tol
  OVERLAP TANGENTIAL TOLERANCE = <real>over_tang_tol
  FRICTION MODEL = <string>friction_model_name|
    FRICTIONLESS(FRICTIONLESS)
  AUTOMATIC KINEMATIC PARTITION
  INTERACTION BEHAVIOR = <string>SLIDING|
    INFINITESIMAL_SLIDING|NO_INTERACTION(SLIDING)
END [INTERACTION <string>name]

# end enforcement

# END [CONTACT DEFINITION <string>name]
# Results specification

BEGIN RESULTS OUTPUT <string>results_name
  DATABASE NAME = <string>results_file_name
  DATABASE TYPE =
    <string>database_type(exodusII)
  OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
    (ON|TRUE|YES)
  TITLE <string>user_title
  NODE VARIABLES = <string>variable_name
    [AS <string>dbase_variable_name] ... 
    <string>variable_name [AS 
    <string>dbase_variable_name]
  | NODAL VARIABLES = <string>variable_name
    [AS <string>dbase_variable_name] ... 
    <string>variable_name [AS 
    <string>dbase_variable_name]
  NODESET VARIABLES = <string>variable_name
    [AS <string>dbase_variable_name] ... 
    <string>variable_name [AS 
    <string>dbase_variable_name]
  | NODESET VARIABLES = <string>variable_name
    [AS <string>dbase_variable_name]
    INCLUDE|ON|EXCLUDE <string list>nodelist_names
    ... <string>variable_name
    [AS <string>dbase_variable_name] INCLUDE|ON|EXCLUDE 
    <string list>nodelist_names
  FACE VARIABLES = <string>variable_name
    [AS <string>dbase_variable_name] ... 
    <string>variable_name [AS 
    <string>dbase_variable_name]
  | FACE VARIABLES = <string>variable_name
    [AS <string>dbase_variable_name]
    INCLUDE|ON|EXCLUDE <string list>surface_names
    ... <string>variable_name
    [AS <string>dbase_variable_name] INCLUDE|ON|EXCLUDE 
    <string list>surface_names
  ELEMENT VARIABLES = <string>variable_name
    [AS <string>dbase_variable_name] ... 
    <string>variable_name [AS 
    <string>dbase_variable_name]
  | ELEMENT VARIABLES = <string>variable_name
    [AS <string>dbase_variable_name]
    INCLUDE|ON|EXCLUDE <string list>block_names
    ... <string>variable_name
    [AS dbase_variable_name] INCLUDE|ON|EXCLUDE 
    <string list>block_names
OUTPUT MESH = EXPOSED_SURFACE|BLOCK_SURFACE
COMPONENT SEPARATOR CHARACTER = <string>character|NONE
GLOBAL VARIABLES = <string>variable_name
  [AS <string>dbase_variable_name] ...
  <string>variable_name [AS
  <string>dbase_variable_name]
START TIME = <real>output_start_time
TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
AT TIME <real>time_begin INCREMENT =
  <real>time_increment_dt
ADDITIONAL TIMES = <real>output_time1
  <real>output_time2 ...
AT STEP <integer>step_begin INCREMENT =
  <integer>step_increment
ADDITIONAL STEPS = <integer>output_step1
  <integer>output_step2 ...
TERMINATION TIME = <real>termination_time_value
USE OUTPUT SCHEDULER <string>scheduler name
OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
  SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
  SIGKILL|SIGILL|SIGSEGV
END [RESULTS OUTPUT <string>results_name]

# User output

BEGIN USER OUTPUT
  # {mesh-entity set commands}
  NODE SET = <string_list>nodeset_names
  SURFACE = <string_list>surface_names
  BLOCK = <string_list>block_names
INCLUDE ALL BLOCKS
REMOVE NODE SET = <string list>nodelist_names
REMOVE SURFACE = <string list> surface_names
REMOVE BLOCK = <string list>block_names
#
# compute global result command
COMPUTE GLOBAL <string>results_var_name AS
  <string>SUM|AVERAGE|MAX|MIN OF <string>NODAL|
  ELEMENT <string>value_var_name
  [(<integer>component_num)]
#
# user subroutine commands
NODE SET SUBROUTINE = <string>subroutine_name |
  SURFACE SUBROUTINE = <string>subroutine_name |
  ELEMENT BLOCK SUBROUTINE = <string>subroutine_name
SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
SUBROUTINE REAL PARAMETER: <string>param_name
SUBROUTINE INTEGER PARAMETER: <string>param_name
    = <integer>param_value
SUBROUTINE STRING PARAMETER: <string>param_name
    = <string>param_value
#
# copy command
COPY ELEMENT VARIABLE <string>ev_name TO NODAL VARIABLE <string>nv_name
#
# compute for element death
COMPUTE AT EVERY TIME STEP
#
# additional command
ACTIVE PERIODS = <string list>period_names
END [USER OUTPUT]

# Time step initialization

BEGIN TIME STEP INITIALIZATION
    # (mesh-entity set commands)
    NODE SET = <string_list>nodeset_names
    SURFACE = <string_list>surface_names
    BLOCK = <string_list>block_names
    INCLUDE ALL BLOCKS
    REMOVE NODE SET = <string list>nodelist_names
    REMOVE SURFACE = <string list> surface_names
    REMOVE BLOCK = <string list>block_names
    #
    # user subroutine commands
    NODE SET SUBROUTINE = <string>subroutine_name |
        SURFACE SUBROUTINE = <string>sub_name |
        ELEMENT BLOCK SUBROUTINE = <string>sub_name
    SUBROUTINE DEBUGGING OFF | SUBROUTINE DEBUGGING ON
    SUBROUTINE REAL PARAMETER: <string>param_name
        = <real>param_value
    SUBROUTINE INTEGER PARAMETER: <string>param_name
        = <integer>param_value
    SUBROUTINE STRING PARAMETER: <string>param_name
        = <string>param_value
    #
    # additional command
    ACTIVE PERIODS = <string list>period_names
END TIME STEP INITIALIZATION

# User variable
BEGIN USER VARIABLE <string>var_name
   TYPE = <string>NODE|ELEMENT|GLOBAL
       [<string>REAL|INTEGER LENGTH = <integer>length]|
       [<string>SYM_TENSOR|FULL_TENSOR|VECTOR]
   GLOBAL OPERATOR = <string>SUM|MIN|MAX
   INITIAL VALUE = <real list>values
   USE WITH RESTART
END [USER VARIABLE <string>var_name]

# History specification

BEGIN HISTORY OUTPUT <string>history_name
   DATABASE NAME = <string>history_file_name
   DATABASE TYPE =
       <string>database_type(exodusII)
   OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
       (ON|TRUE|YES)
   TITLE <string>user_title
   #
   # for global variables
   VARIABLE = GLOBAL
       <string>variable_name
       [AS <string>history_variable_name]
   #
   # for mesh entity - node, edge, face,
   # element - variables
   VARIABLE =
       NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
       AT NODE|NODAL|EDGE|FACE|ELEMENT <integer>entity_id
       [AS <string>history_variable_name]
   #
   # for nearest point output of mesh entity - node,
   # edge, face, element - variables
   VARIABLE =
       NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
       NEAREST LOCATION <real>global_x,
       <real>global_y>, <real>global_z
       [AS <string>history_variable_name]
 START TIME = <real>output_start_time
 TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
 AT TIME <real>time_begin INCREMENT =
       <real>time_increment_dt
 ADDITIONAL TIMES = <real>output_time1
       <real>output_time2 ...
 AT STEP <integer>step_begin INCREMENT =
       <integer>step_increment
 ADDITIONAL STEPS = <integer>output_step1
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<integer>output_step2 ...
TERMINATION TIME = <real>termination_time_value
USE OUTPUT SCHEDULER <string>scheduler_name
OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|
SIGINT|SIGHUP|SIGQUIT|SIGTERM|
SIGUSR1|SIGUSR2|SIGABRT|
SIGILL|SIGSEGV
END [HISTORY OUTPUT <string>history_name]

# Heartbeat specification

BEGIN HEARTBEAT OUTPUT <string>heartbeat_name
# Can also use predefined streams "cout", "stdout",
# "cerr", "clog", "log", "output", or "outputP0"
STREAM NAME = <string>heartbeat_file_name
#
# for global variables
VARIABLE = GLOBAL
<string>variable_name
[AS <string>heartbeat_variable_name]
#
# for mesh entity - node, edge, face,
# element - variables
VARIABLE =
NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
AT NODE|NODAL|EDGE|FACE|ELEMENT <integer>entity_id
[AS <string>heartbeat_variable_name]
#
# for nearest point output of mesh entity - node,
# edge, face, element - variables
VARIABLE =
NODE|NODAL|EDGE|FACE|ELEMENT <string>variable_name
NEAREST LOCATION <real>global_x,
<string>global_y>, <real>global_z
[AS <string>heartbeat_variable_name]
START TIME = <real>output_start_time
TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
AT TIME <real>time_begin INCREMENT =
<string>time_increment_dt
ADDITIONAL TIMES = <real>output_time1
<string>output_time2 ...
AT STEP <integer>step_begin INCREMENT =
<string>step_increment
ADDITIONAL STEPS = <integer>output_step1
<string>output_step2 ...
TERMINATION TIME = <real>termination_time_value
USE OUTPUT SCHEDULER <string>scheduler_name
OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
SIGKILL|SIGILL|SIGSEGV
PRECISION = <integer>precision
LABELS = <string>OFF|ON
LEGEND = <string>OFF|ON
TIMESTAMP FORMAT <string>timestamp_format
MONITOR = <string>RESULTS|RESTART|HISTORY
END [HEARTBEAT OUTPUT <string>heartbeat_name]

# Restart specification

BEGIN RESTART DATA <string>restart_name
    DATABASE NAME = <string>restart_file_name
    INPUT DATABASE NAME = <string>restart_input_file
    OUTPUT DATABASE NAME = <string>restart_output_file
    DATABASE TYPE = <string>database_type(exodusII)
    OVERWRITE = <string>OFF|ON|TRUE|FALSE|YES|NO
    (ON|TRUE|YES)
    START TIME = <real>restart_start_time
    TIMESTEP ADJUSTMENT INTERVAL = <integer>steps
    AT TIME <real>time_begin INCREMENT = <real>time_increment_dt
    ADDITIONAL TIMES = <real>output_time1
    <real>output_time2 ...
    AT STEP <integer>step_begin INCREMENT = <integer>step_increment
    ADDITIONAL STEPS = <integer>output_step1
    <integer>output_step2 ...
    TERMINATION TIME = <real>termination_time_value
    OVERLAY COUNT = <integer>overlay_count
    CYCLE COUNT = <integer>cycle_count
    USE OUTPUT SCHEDULER <string>scheduler_name
    OUTPUT ON SIGNAL = <string>SIGALRM|SIGFPE|SIGHUP|SIGINT|
    SIGPIPE|SIGQUIT|SIGTERM|SIGUSR1|SIGUSR2|SIGABRT|
    SIGKILL|SIGILL|SIGSEGV
END [RESTART DATA <string>restart_name]

END [PRESTO REGION <string>presto_region_name]

END [PRESTO PROCEDURE <string>presto_procedure_name]

END [SIERRA <string>name]
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