Computational Mechanics

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Thrust Area Leader

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An aerial, grayscale photograph of a city grid, likely Los Angeles, showing a dense pattern of streets and buildings. The image is used as a background for the report cover.

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The Computational Mechanics thrust area has continued to sponsor investigations into the solid, structural, and fluid mechanics and heat transfer underlying the state-of-the-art computational software used in engineering analysis in support of programs at Lawrence Livermore National Laboratory (LLNL).

The scale of capability spans the office workstation and its continued expansion of interactive and graphic capability, to "departmental" or building compute servers, and finally, central or national massively parallel supercomputing. Our past breadth in technology transfer to industry has narrowed, and is focused toward funded activity.

The Department of Defense High Performance Computing and Modernization Program is funding the LLNL ParaDyn Project to port DYN3D to their major resource centers. The DOE Defense Program's ASCI Blue acquisition holds ParaDyn as one of its prototype applications. In addition, the Federal Aviation Agency is funding LLNL to provide DYN3D (and eventually ALE3D) to the aircraft industry as a toolkit to address debris damage and mitigation assessment.

This past year has been the first full year that the Methods Development Group (MDG) has been under the leadership of P. Raboin, who has written a survey article on code activities, including general DYN3D, NKE, and TOPAZ enhancements, as well as mesh generation and graphic post-processing tools. C. Hoover presents an article on the overall ParaDyn Project, with her broad team and many activities. J. Lin and M. Puso each have articles on new rigid body material options just added to DYN3D and NKE3D, respectively. All of these activities are within the MDG, and together with P. Raboin's article will be expanded into a special code capabilities document.

Additional articles this year include the effort led by A. Shapiro to characterize the laser-induced mechanical failure and damage of optical components; creative use of a suite of heat transfer codes to perform a thermal evaluation of the nuclear weapons pit storage facility at Pantex, by B. Komblum; radiation-induced thermal stresses in high-power flashlamps, by J. Malby; and finally, the simulation of turbine fragment containment and mitigation of aircraft engines, by G. Kay and E. Zywicki.

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Finite-Element Code Enhancement

Peter J Raboin

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The DYNA, NIKE, TOPAZ, and GRIZ family of finite-element codes provide Lawrence Livermore National Laboratory (LLNL) programs (50-60 analysts) with needed dynamic, structural and thermal analyses. Our broad service charter is to provide rapid and highly skilled user support and has resulted in over 75 improvements to these codes in FY-96. Material switching capabilities in DYNA3D and new NASA matrix solvers in NIKE3D have increased the execution speeds of these codes by factors of over 1000, and have permitted heretofore in possibly complex and large finite-element model analyses. Visualization capabilities are expanding with promising developments in the areas of parallel processing, ASCII-compliant standards and plot database flexibility. Exciting new advancements in computer hardware (DEC Alpha and IBM SP2) are quickly being matched with code portings to these new platforms. Web-browsing capabilities for our software manuals were demonstrated for DYNA3D and MAZE this year, with more manuals to follow. Finally, the Code Collaborators Program has been strengthened with tougher standards for admission, renewals and documentation.

Introduction

There are diverse and numerous year-end deliverables for the Methods Development Group (MDG) at LLNL, because of its primary function as a code support, code development, and research organization. Each year within MDG, there are specific projects to add larger code capabilities to our software. For example, the ParaDyn project is adding parallel capabilities, and another project adds rigid body capabilities to DYNA3D and NIKE3D.

In FY-96, our code enhancement work consisted of five projects: DYNA, NIKE, TOPAZ, pre- and post-processing and rezoning. This report describes some of the general code up-grades, gives short descriptions of the major accomplishments for each project, and provides a Code Collaborators Program status update.

A more detailed listing of the specific code enhancements for FY-96 is given in an appendix.

Progress

General Up-grades

During FY-96, up-grades in computer equipment and operating systems had a broadening effect on the base of MDG code development. Sun Solaris operating systems were added across LLNL, and

new DEC Alpha machines were purchased for open and classified computing. The MDG codes were ported to support these changes.

At present, our serial codes support the following platforms: Cray, DEC Alpha, HP, IBM RS6000, SGI, and Sun. We support multiple hardware and operating system variations for several of these machines. Executables for these codes are maintained on both the open and classified computing systems. The supported parallel machines are Meiko, Cray T3d, and IBM SP2. Concurrent Version System (CVS) version control is used to provide single-source code tracking and to facilitate multiple code developer activities.

During the last months of FY-96, the MAZE and DYNA3D manuals appeared for the first time as Web HTML documents. This was accomplished with a software package that converts FrameMaker documents to HTML. Formal requests have been made to provide NetScape on LLNL's classified system so that these manuals may be interactively viewed. It is our intention to provide up-to-date manuals via this medium for all of the MDG codes on the unclassified and classified systems.

DYNA

Mixed-time integration methods, contact algorithms and user-requested code improvements were

important priorities in this year's MDG DYNA3D development. Two rigid body features, improved rigid body joints and deformable/rigid material switching were also added. The implementation strategy for mixed-time integration is laid out. Element/node partition work is in progress. The sub-cycling scheme will be implemented with selected contact types in the coming year.

Two contact capabilities were improved: tying SAND into type-8 contact, and adding automatic contact velocity damping for Lagrange projections. User-requested DYNA improvements aided the AT-400A (Fig. 1), W56 Transportation Safety Risk Assessment (TSRA), FL Container, and DOD penetrator studies in the Defense Technologies Engineering Division (DTEd). Work performed for Energy Manufacturing and Transportation Technology (EMATT) by the New Technologies Engineering Division (NTEd) was helped with features added to assist the VM and Composites Cooperative Research and Development Agreements (CRADAs) and the Boeing project. Another important accomplishment this year was the preparation and presentation of a DYNA3D training course.

Figure 1. The AT400A transportation container, experimentally and analytically dropped, crushed, and cooked to validate and prove its functionality as a transportation container for nuclear weapon components

NIKE

For NIKE3D development, the top priorities were up-grades to the structural elements, improved linear solvers, double precision, a short effort in NIKE-DYNA-NIKE linkages, and user-requested code improvements. These goals were largely achieved. There are now concrete shell and beam models for structural elements, user-defined integration for concrete and windshield composites, and a new membrane element for metal forming.

Two new linear solvers were added and a double precision version of NIKE3D was completed for workstation use. A linkage capability was also demonstrated and used to motivate the element technology Laboratory-Directed Research and Development (LDRD) proposal. Two Lasers Program projects benefited this year from NIKE3D development: a NIKE3D coupling to thermo-optical diffraction calculations and another NIKE3D coupling to a commercial multiple-optic beam path calculation code (TSO). Special assistance was provided for the Boeing CRADA (in NTEd) with additions of the membrane element and added capabilities for the Super Plastic Forming pressure scheduler. The FL container vibration problem (in DTEd) benefited from close user support and two new capabilities: NASA's variable band solver (VBS) and an auto-time-stepping algorithm for dynamic vibration problems (Fig. 2).

TOPAZ

Based on programmatic requests (from DTEd) and the prevalence of computer workstations, a double precision version of TOPAZ3D was created this year. This work, which affects data structures and I/O routines, was made compatible with the new double precision version of NIKE3D. This was done to simplify the future integration/up-grade of these codes into the coupled NIKE3D code. This latter code was ported in FY-96 from the workstation to the Cray J-90 supercomputer.

FACET was also up-graded in FY-96 by implementing the more accurate axisymmetric radiation view factor algorithm from the GLAM physics code. GLAM was written in the late 1970's on the CDC7600 using LRLTRAN.

Pre- and Post-Processing

The GRZ post-processor was our top priority in FY-96. Its development is central to the ParaDyn effort and to our goals in supporting the new LLNL

ASCI Program. We are a member of the ASCI Common Data Format Working Group, the goal of which is to create a common (portable) scientific data file format/Application Program Interface (API) to support ASCI work. In conjunction with our goals for GRIZ and our participation in ASCI, the mesh input/output (Mili I/O) library received considerable development this year as a replacement to the fixed TAURUS database. The Mili I/O library has both C and Fortran interfaces that will be used by the analysis codes and GRIZ. Completion of the Mili library interface is now proceeding, in conjunction with the conversion of GRIZ to a mesh I/O based (Mili) application.

For pre- and post-processing in general, we have completely revamped three manuals, for GRIZ, THUG, and MAZE. Running GRIZ on Sun workstations was finally accomplished this year. The latest Ultra-Sparc workstations have a hardware graphic OpenGL capability, and the older Sparc workstations can use Mesa, a freeware version of OpenGL. GRIZ is now functional on all of the MDG supported platforms and its use by the analysts is increasing. The addition of THUG as a specialized time-history graphical program has bridged all of the capabilities of TAURUS.

GRIZ and THUG supported important programmatic and research work this year with new time-history filtering features for the AT400A impact analyses, advanced iso-surface visualization capabilities for the Array of Conventional Explosives (ACE) project and unique feature support of the Large Eddy Simulation (LES) turbulence modeling LDRD.

Minimal support was maintained for Orion and Ingrid in FY-96. A low level of support is anticipated for MAZE in FY-97. With a new MAZE manual and the addition of a repertoire of region commands, the FY-97 feature requests for MAZE are limited. Animation activities were in strong demand this year (21 high quality videos were produced). MDG continues to support a modest video creation capability, and new animation capabilities were added with the purchase of advanced visualization capabilities through WaveFront.

Rezoner

A new 3-D rezoning task was initiated this year with three goals: 1) graphical monitoring of the analysis results while the code is running; 2) interactive rezoning between analysis iterations; and 3) automatic rezoning between iterations, either through scripting or error detections. This was to be a multi-year phased project, but a departure of

key personnel in FY-96 has forced suspension until suitable replacements are identified. Completed this last year is a software development design plan that investigated user requirements and compatibility between analysis codes, GRIZ, and the rezoner requirements. We completed work on interfaces for 3-D interactive rezoning and also demonstrated a prototype capability to display mesh quality measures (skewness and aspect ratio) in GRIZ.

Code Collaborators Program

The Code Collaborators Program this year saw the addition of 32 new collaborators (32 renewals) and the dropping of old collaborators who had

Figure 2. The FL container, subjected to extensive vibration analyses with NIKE3D to study its overall mechanical response and the structural integrity of certain welded joints

shown no participation in the last 18 months. The program currently has 152 collaborators, consisting of 54 academic institutions, 72 industrial partners, 21 government organizations, and 5 associates who have legal partnerships with LLNL. Following DOE requirements, the Energy Science and Technology Software Center (ESTSC) was up-dated this year with copies of our most recent "stable" software. The ESTSC meets the needs of those interested in obtaining our codes for analysis, thereby decreasing the demands placed on the program, while retaining those organizations who truly pursue code development.

The purpose of collaboration remains the same: we wish to advance the development of MDG codes through the mutual sharing of software developments, bug fixes, and general capability enhancements. Several notable code contributions were obtained this year. A new NASA solver was incorporated into NIKE3D. This solver was essential in solving a FL container vibration problem for DTED. It provided a 6500% code speed-up using four times less memory. Logicon gave us a new material model (#45) which is an enhancement of model #16 for geologic materials. The Defense Evaluation Research Agency in the UK provided complete copies of their source up-dates as well as their documentation for ISO 9003 software quality assurance registration of DYNA3D software.

There remains a back-log of unincorporated collaborator contributions that are prioritized by the LLNL community needs. This program remains valuable for the capability improvements and bug fixes we receive.

Summary

The MDG group activities affect a large user base of 50 to 60 analysts who are principally in the DTED, NTED and Laser divisions of Mechanical Engineering at LLNL. In FY-96, the MDG code development projects were aligned with the codes that require the most support and receive the greatest use. Most interactions between the code developers and the users are brief, being either quick feature enhancements or bug reports with subsequent fixes. Not shown in this report are the day-to-day user interactions of instruction, model debugging, and problem brainstorming which often go into solving difficult solid mechanics and heat transfer problems. The Code Collaborators Program has continued this year with tougher participation requirements and an increased reliance on the ESTSC for satisfying demands for "public domain" versions of DYNA, NIKE, and TOPAZ software.

Future Work

Since the numerous code capability improvements undertaken by MDG in FY-96 were motivated by the user community, a prediction of future work is difficult.

What is known is that the Cray J-90's will get an operating system up-grade, which means that Fortran 90 modifications are needed for all of MDG codes. Element technology research will provide greater mid-analysis switching capabilities between DYNA3D and NIKE3D, compatible DYNA3D/NIKE3D element formulations and more stable element formulations.

Parallel developments undertaken by the ParaDyn project will deliver more computing horsepower to the analyst than ever before, so more MDG user support is expected in this area. DYNA3D work continues on sub-cycling, contact improvements, and rigid body joint failure. NIKE3D work will improve implicit dynamics (HHT integration), rotational inertia for shells, and beams, and modal superposition. Incorporation and merging of the GEMINI capabilities into NIKE3D is also planned. TOPAZ3D expects to improve its shell element heat transfer capabilities as well as implement some of the new matrix solver routines. Continued GRIZ development is focused on Mili, parallel implementations, and a substantial user request list.

Web browsing for our manuals is seen as a necessary task to bring MDG documentation up to current technology standards. Finally, more effort is being directed to quality assurance improvements in our conduct of code development.

Appendix

The lists in this section are for individual codes that received Computational Mechanics Thrust Area funding in FY-96. Items indicated by $\diamond$ are purely LLNL activities; those marked with an asterisk (*) are external collaborator contributions.

DYNA3D

New and Improved Features

- $\diamond$ Material switching
- $\diamond$ Revolute joints
- $\diamond$ Dynamic memory allocation
- $\diamond$ Velocity correction to Lagrangian contact algorithm
- $\diamond$ Mass proportional damping switch (on/off)
- $\diamond$ Command line file sizes
- $\diamond$ Volumetric strain failure criterion added to material type 11

- ◊ Composite material orientation
- * Material model #45: improved material type 16
- ◊ Material model #46: fully anisotropic elasticity
- ◊ Multiple type-2 load curves
- * Type-8 slide surfaces in SAND
- ◊ Additional NIKE3D to DYNA3D stress initialization options
- ◊ One-step plane stress elastoplasticity algorithm added
- ◊ Bathe-Dworkin and fully-integrated YASE shell element formulations
- ◊ Slave node radii in type-5 contact—discrete nodes impacting a surface
- ◊ Model #22 minimum time-step size deletion criteria, plus additional failure options
- ◊ Multiple groups of materials for Rigid/Deformable Material Switching
- ◊ Breakable Rigid Body Joints with activation time and acceleration failure criterion
- ◊ User-defined initial velocity superposition for rotational motion
- ◊ Suppression of SAND failure information in printout

Bug Fixes

- ◊ Internal energy for discrete spring/damper elements
- ◊ Hughes-Liu shell element
- ◊ Rigid Body Joints error in initial position differences
- * Vectorized auto contact
- ◊ Tie-Breaking Shell Slidelines
- ◊ Deformable/Rigid Material Switching
- ◊ Thick shell elements
- ◊ Equation of state 11

DYNA2D

Bug Fixes

- ◊ TOPAZ2D plotfile compatibility
- ◊ Double precision bugs in common blocks

NIKE3D

New and Improved Features

- ◊ Makefile
- ◊ Viscoelasticity material model
- ◊ 24-point limitation for user-defined beam and shell integration points eliminated
- ◊ Concrete damage and cyclic steel plasticity beam model
- ◊ Double precision
- ◊ Compressed row format storage of stiffness matrix

- * Cray Research Inc. VBS solver
- * SGI and HP Sparse Solvers
- ◊ Additional time-history and incompatible modes output
- ◊ Membrane element
- ◊ Bisection (line search) algorithm for SPF pressure scheduler
- * NASA VSS solvers
- ◊ Dynamic memory allocation
- ◊ Auto-time-stepping algorithm, called AUTV, to solve dynamic vibration
- ◊ Improved tangent stiffnesses for contact
- ◊ Single pass contact and improved search algorithms

Bug Fixes

- ◊ Thermomechanical double precision
- ◊ Memory holes in dynamic memory allocation for HP workstations
- ◊ File size mismatches with TOPAZ3D
- ◊ Slide surface memory conflicts with rigid body data structures
- ◊ New FL input format

NIKE2D

New and Improved Features

- ◊ GRIZ plot format
- ◊ Interference fits for slide lines

Bug Fixes

- ◊ Double precision load curves
- ◊ Zero load application error

TOPAZ

New and Improved Features

- ◊ Added logic to reduce the time step if the stiffness matrix is non-positive definite
- ◊ Replaced variable time step coding in TOPAZ3D with more robust coding from TOPAZ2D
- ◊ Double precision

Bug Fixes

- ◊ Corrected bug in dump/restart subroutines—the number of words in a common block was incorrectly defined.
- ◊ Corrected bug in slide line logic (a crash occurred when the user specifies 0 for the contact conductance). This is now captured and the slide line is ignored.
- ◊ Corrected bug in dump/restart logic (if for the last time step may be 0 or very small so that the end time is hit exactly).

- ◊ Fixed bug in reading an exchange factor text file. The exchange factor matrix is non-symmetric. The previous coding read a symmetric view factor matrix.
- ◊ Unresolved FEM formulation problem. A NIF problem showed an anomalous negative temperature wave moving through the mesh. No bug could be found in TOPAZ. The commercial code ANSYS gave the same anomalous results.

GEMINI

New and Improved Features

- ◊ Composite nodal damping
- ◊ Workstation version
- ◊ Repetitive bad case generation

Bug Fixes

- ◊ Corrected bandwidth minimization for shells having composite nodal damping

GRIZ

New and Improved Features

- ◊ Updated GRIZ manual to 2.0
- ◊ Unit conversion via scale and intercept
- ◊ Material manager material selection picking
- ◊ "tellpos" node/element position queries via command line mouse picking
- ◊ Refined color legend and scaling procedure
- ◊ GRIZ under HP/UX using Mesa on an HP workstation
- ◊ GRIZ on the Dec Alpha
- ◊ Automatic length determination for floating point displays in time-history plots
- ◊ Mesh bounding box updates
- ◊ Mode-dependent cursor shapes
- ◊ Dynamic linking to user-defined libraries of time-series transformation functions
- ◊ Multiple independent sets of particle traces
- ◊ Save/restore of particle traces
- ◊ Disable particle traces for selected materials
- ◊ Save vector field values
- ◊ Node-base vector fields

Bug Fixes

- ◊ Material manager GUI
- ◊ Interpolated time display
- ◊ Y-axis labeling for time-history plots
- ◊ Time-history re-calculation after a change in the basis, reference surface, or strain variety
- ◊ Ensure that edge lines are rendered on top of coincident polygons
- ◊ TOPAZ3D plotfile database compatibility

Mili I/O

New and Improved Features

- ◊ Mili allows per-subrecord data organization so that either object-ordered or results-ordered data structures can be used.
- ◊ Mili has a memory management layer for facilitating the traversal and re-organization of internal data structures.
- ◊ Mili can detect an "active" database and is able to operate on a growing database.
- ◊ Mili has added the data structures (hash tables) to support derived and primal results and GRIZ is similarly supporting dynamic menu creation.

THUG

New and Improved Features

- ◊ Interpreted "sum" and "diff" commands for derived results
- ◊ thd2s utility added to convert Cray to Workstation data formats
- ◊ Dynamic linking to user-defined libraries of time-series transformation functions
- ◊ Nodal data exclusion flag for time-history database
- ◊ Incorporated Low-Pass Butterworth digital filter
- ◊ Up-dated the THUG User Manual
- ◊ Completed THUG software distribution for the Code Collaborators Program

MAZE

New and Improved Features

- ◊ Expanded region command capabilities
- ◊ Completed a new User's Manual
- ◊ New slideline types supported
- ◊ Equation-of-state modifications
- ◊ Region node number assignment to a parameter symbol

ANIMATION

- ◊ Tiling modifications to "Advanced Hydro Test Facility" (J. Pastmak)
- ◊ "Pulse-Induced Deformation in a Laser Slab" (M. Rotter)
- ◊ Shortened "Computational Biomechanics" (for G. Goudreau)
- ◊ "Large Eddy Simulation of Flow Over a Backward Facing Step" (B. Kornblum and R. McCallen)
- ◊ "GM Casting Rework" (P. Raboin)
- ◊ "ParaDyn Benchmark Applications" (C. Hoover and T. Degroot)

- ◇ "The Role of Animation Production in Visualization" (M. Loomis)
- ◇ "High-Bypass Commercial Aircraft Engine Simulation" (E. Zywicki)
- ◇ "Vector Carpets for Irregular Grids" (D. Dovey)
- ◇ "Earthquake Simulation Compilation" (D. McCallen and T. Chargin)
- ◇ "Finite Element Modeling of Lower Extremities" (S. Perfect)
- ◇ "TEAM Virtual Manufacturing: Sheet Metal Forming" (T. Lee)
- ◇ "LLNL High Performance Computing" (G. Goudreau, J. Peters (NASA))
- ◇ "Large Eddy Simulation of Turbulent Separating Flow" (B. Komblum and R. McCallen)
- ◇ "Computational Biomechanics at LLNL" (K. Hollerbach and D. Schauer)
- ◇ "Spin-Forming of Uranium Components" (P. Raboin)
- ◇ Presentation graphics (transparency and paper hardcopy) (for H. Louis)
- ◇ Copies of "Seismic Response of the 24-580-980 Interchange" (D. McCallen)
- ◇ "Array of Conventional Explosives In Use Against a Deep Target" (D. Badders and M. Shannon)
- ◇ "Laminar Backward-Facing Step Flow" (B. Komblum)
- ◇ "Arrays of Conventional Explosives in Use Against a Deep Tunnel" (D. Badders)
- ◇ Presentation graphics (transparency and paper hardcopy) (for G. Bernal)
- ◇ "DYNA3D Model of AT400A Drop Tests" (D. Badders)
- ◇ "OAB-LTAB Material Flow Animation" (M. McDaniel)

Parallel Algorithm Research for Solid Mechanics Applications Using Finite Element Analysis

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The goal of this project is parallel algorithm development for both explicit and implicit finite element applications in solid and structural mechanics. New capabilities developed this year include the development of software modules for multiple partitioning of the finite element meshes, efficient parallel implementation of mechanics algorithms in DYNA3D, and production simulations of underground shock-structure interactions with over a million elements. Performance results for ParaDyn, the parallel version of DYNA3D, demonstrate parallel scalability and efficiency for several benchmark applications and production problems.

Introduction

This research in parallel algorithms is targeted for the two nonlinear, large deformation solid mechanics programs, DYNA3D and NIKE3D. DYNA3D¹ is an explicit finite-element program for analyzing the transient dynamic response of 3-D solids and structures. The element formulations available include 1-D truss and beam elements, 2-D quadrilateral and triangular shell elements, and 3-D continuum elements. The thirteen contact-interface algorithms provided in DYNA3D include state-of-the-art algorithms for modeling arbitrary contact for large deformations, frictional sliding, single surface contact, and contact with failure. Rigid materials provide added modeling flexibility.

NIKE3D² is a fully implicit finite element program for analyzing the finite-strain, static response of 3-D solids and structures. Spatial discretization includes solid, shell, beam and truss elements with 8-point, 4-point and 2-point integration for these element types. Four contact interface algorithms permit gaps, frictional sliding, and mesh discontinuities along material interfaces. The resulting system of simultaneous linear equations is solved either iteratively using an element-by-element method, or directly by a factorization method. Nonlinear solution strategies include full-, modified- and quasi-Newton methods.

DYNA3D (ParaDyn) uses a successful strategy for parallel implementation of an explicit finite element method^{3,4} based on dividing the finite element mesh among the processors and executing ParaDyn on the individual subdomains. This is a message-passing parallel model with nodal point data identified as the shared data between processors. The challenging aspects of the parallel algorithm development are the optimal partitioning of the finite element mesh and the treatment of the interfaces at material boundaries (contact algorithms). Reference 4 describes a benchmark application in crashworthiness simulations.

Current research⁵ in graph partitioning algorithms provides a means for developing automated tools for partitioning finite element meshes. It is now possible to develop multiple partitions for domains based on a physical partitioning of the problem as well as for treating boundary conditions such as contact. Software development for automating multiple partitioning methods is described in a section below. These methods can be extended into parallel form as needed for future large applications.

Parallel computers today are characterized by their memory hierarchy as well as by the number of processors on the full system. Typically, the number of processors varies from as few as 8 to as many as 4,000. For computers with a large number of processors, the memory is always distributed with an

interconnect network between individual nodes. The nodes may include multiple processors that share cache and secondary memory. The parallel programming model in this case is generally message-passing.

The smallest parallel computers are typically a single node with processors sharing the memory by means of a high-speed bus interconnect. Although in the past the parallel programming model for these computers has been shared memory, the emergence of the Message Passing Interface (MPI) standard has provided shared memory computer vendors the motivation and impetus to provide this programming model as well. Future parallel computers are expected to include shared memory nodes with an interconnect network. The implementation of the MPI standard in ParaDyn in this last year, along with optimal mesh partitioning, will enable efficient problems on future parallel computers regardless of their architecture.

Research leading to parallel algorithms for NIK3D is just beginning. The plan for implementing parallel algorithms in NIK3D is to develop first a shared memory version of linear solvers for an 8- to 10-fold increase in problem performance for a minimum amount of reprogramming effort. This will enable longer time simulations for applications such as spin-forming in the near future. Current research efforts are being directed toward message-passing solution techniques that will enable the larger size NIK3D applications on the next generation massively parallel computers.

Figure 1. Underground blast simulation modeled with over seven million degrees of freedom.

Progress

The most notable accomplishments in FY-96 have been (1) the simulation of problems with over a million elements; (2) simulations of large underground shock/structure problems with localized contact; and (3) the development of parallel algorithms to implement the mechanics capabilities needed for production applications and parallel benchmark tests.

Parallel Applications and Performance

One of our most challenging goals has been to demonstrate a production ParaDyn calculation with up to a million elements. The calculation shown in **Fig. 1** is one of a series of underground blast calculations simulated on a 128-node Meiko CS-2, and more recently on a 256-processor IBM SP-2. The problem sizes vary from a million elements to several million elements, and demonstrate excellent scaling for the Meiko CS-2, the IBM SP-2, and the Cray Research Incorporated T3D, as shown in **Fig. 2**. A series of performance studies using 128 Meiko nodes with two processors per node resulted in roughly 50% improvement over the results using one processor per node. The absolute performance on the SP-2 using 128 processors is 5 μ s per element cycle. This is roughly 50 times faster than a single processor on a Cray YMP.

Figure 2. Performance of parallel computers. The performance measurements are based on automatic optimization provided by the compilers. No machine-dependent changes were made to the ParaDyn source program.

Last year a collaborative activity with researchers at the Waterways Experiment Station in Mississippi was initiated through the Department of Defense High Performance Computing and Modernization Program. **Figure 3** is the first of several production benchmarks problems which are deliverables to demonstrate parallel performance. This benchmark is a simulation of an underground shock/structure interaction. The contact surfaces between the soil and the structure were modeled with the nodes-in-processor contact algorithm.^{3,4} The contact included one tied surface and five surfaces modeled with a symmetric penalty algorithm. New preprocessing software, described below, was developed to partition the contact surfaces.

Validation of results on parallel computers is an important component of this project. **Figure 4** illustrates a benchmark application that is a robust test of the parallel automatic contact algorithm and that provides an interesting physical system for studying nonlinear phenomena and fractal power laws. The dynamics of the crumpled surface shown in the figure is modeled by compressing a thin sheet with six moving stonewall boundaries. This simulation is run for many sound traversal times and the calculation time is significantly affected by the contact search and force calculations. The large number of contacts at high compression make this a severe test for verifying that all contact points are located and that parallel implementation is correctly summing the contact forces on all processors with shared nodes.

The design of production parallel runs on a routine basis requires characterizing the performance of individual parallel algorithms in ParaDyn to provide guidelines to the analyst for selecting an optimal number of processors for the algorithms used in a particular application. Current performance results show that problems composed primarily of solid elements will perform efficiently with roughly 1000 elements allocated in a processor. In contrast, applications dominated by shell elements, such as the simulations of automobile crashworthiness, perform efficiently with as few as

Figure 3. Underground shock/structure interaction at the end of the calculation. The right wall and the right portions of the back wall, ceiling and floor are a reinforced concrete material. The maximum pressure is shown with the darkest shading and the minimum pressure is white. Maximum damage occurs at the center of the right wall.

Figure 4. Thin square sheet of shell elements compressed by six moving stonewall boundaries which form the faces of a cube. The boundaries are moving at a speed slow compared to the sound speed of the material so that the initial pressure is small compared to the yield strength. The nonlinear folding of the material provides a very robust test of the contact algorithms.

250 elements in a processor. The nodes-in-processor algorithm used for the 21 contact surfaces in the crashworthiness simulation described in Reference 4 can become inefficient if the partitioning of the elements produces a significant number of shared nodes in each processor. We are adapting the preprocessing software to prevent this. In particular, contact surface pairs can be allocated fully within one processor or a subset of the processors. Progress described below on the preprocessing software is a major step toward reaching this result.

ParaDyn Algorithms

An important emphasis of the work this year has been the implementation of mechanics capabilities needed for parallel production applications. Parallel and serial versions of DYN3D and ParaDyn have been merged into a single source. Parallel versions of the Hughes-Liu shell, applied loads (pressure loads, nodal forces, base accelerations), non-reflecting boundary conditions and rigid body mechanics

have been completed. Work is in progress on the parallel automatic contact algorithm to complete the implementation of new features such as material inclusion/exclusion and boxes defining the portion of the grid for automatic contact. The new multiple automatic contact algorithm requires the redesign of the parallel data structures and will be continued into next year.

The parallel rigid body algorithm is designed to minimize communication for rigid body motion through the use of efficient parallel global sums and is implemented as follows. The rigid material option in DYN3D (material type 20) transforms the finite elements in the material into the list of nodes representing a rigid body and the physical parameters associated with the rigid body: center of mass coordinates, body velocities and accelerations, the moment of inertia, body forces and constraints. The parallel algorithm for rigid bodies assigns the nodes in a rigid body to processors based on the partitioning for the elements. For a shared node, the processor selected to include the node in its rigid body sums is the processor with the lowest logical processor number.

Figure 5. Load balancing achieved with multiple partitions A partitioning of the boundary elements separate from the remaining elements on the mesh provides a method for load balancing a calculation. (a) Two partitions are used for a penetration mechanics problem assigned to the four processors. The elements in the penetrated material are allocated to four processors and the penetrator elements are allocated to the first two processors. The contact surface boundary conditions are allocated to the first two processors. (b) A fluid/structure interaction calculation uses three partitions, one for the fluid, another for the submarine hull, and a third for the surface elements between the fluid and structure.

For rigid materials communication during the initialization is used to assign the shared nodes to the lowest processor and to search over individually constrained nodes to evaluate body constraints. Global sums are used to compute body parameters so that all processors know these values for every rigid material. The time integration for the rigid nodes, including shared nodes, is carried out knowing the updated rigid body velocity. The advantages of this algorithm are that the partitioning of rigid materials is the same as that for deformable materials and the partitioning can be weighted by the relative cost of the calculations for rigid body motion and deformable mechanics.

Multiple Partitions for Load-Balanced Calculations

Flexible partitioning software is needed to provide multiple partitions based on the physical characteristics of the problem and the need to load-balance a parallel calculation. **Figure 5** illustrates this idea. **Figure 5a** shows a problem using two partitions, the first for the elements and the second for the contact surfaces. The elements are partitioned using an algorithm selected from the METIS software. The contact surfaces are allocated to processors so that each sliding interface is wholly contained in one processor or a subset of the processors.

The second example (**Fig. 5b**) illustrates the partitioning of a mesh for the PING program, a structural acoustics program coupling a wave equation solver in the fluid with an implicit structural analysis of the submarine. The computer time required to impose the boundary condition between the submarine hull and the fluid represents a significant fraction of the total computational time.

To load-balance this calculation it is important to distribute the elements on the boundary among all of the processors. This can be accomplished using three partitions, one for the elements composing the boundary and two others for the elements in the remainder of the problem. Merging the partitions together produces the desired effect of load-balancing the expensive calculations at the boundary with the calculations in the fluid and structure.

The preprocessing software for partitioning a mesh is illustrated in **Fig. 6**. New programs developed in this last year are shown in shaded boxes. These programs automate the partitioning of the boundary conditions and handle all of the special cases (for example, the local contact surfaces and tied node sets). The new programs were developed to automatically treat the sliding interface partitioning

for the underground shock/structure interaction problem described previously. In this problem the elements that form the sliding interfaces between the soil and the structure are all allocated to one processor. The remaining elements in the problem are partitioned using METIS and assigned to other processors. The partitioned results from METIS are merged with elements assigned to the processor for contact calculations using the MERGECOL program. The merged result is used as input to the PFGEN program to produce the partitioned file used as input to ParaDyn.

The following is a brief description of each of the programs used in the partitioning software. Additional details are found in References 3 and 6.

SNPGEN parses the DYN3D input file and extracts the slide surface data and other boundary data needing special treatment in the partitioning of the mesh. The output from SNPGEN is a file containing Special Nodal Point sets. These sets of nodes, one for each boundary condition, are subsequently input to PFGEN to be allocated to processors based on specific rules. One example of a rule is the node-in-processor contact algorithm.

DUALGEN reads the list of nodes and elements in the DYN3D input file and uses efficient algorithms to generate the dual mesh. The dual mesh is the mesh of connected elements. DUALGEN additionally generates a file of Special Element sets using the

Figure 6. Preprocessing software, designed as a collection of tools to be used with several analysis programs. Each tool can be used separately for generating partitions for specific problem meshes, boundary conditions, and analysis programs.

output of SNPGEN. The SpecialElement sets include allelements which have one or more of their nodes in the corresponding SpecialNodalPoint set.

TRANSCLOSE combines SpecialElement sets if the sets share one or more elements. Duplicate elements are removed in the combined set.

SESCOL is a program planned for the future. It will assign processors to the SpecialElement sets developed by TRANSCLOSE.

MERGEOL combines the results from the METIS partitioning with the results from the TRANSCLOSE and SESCOLO programs to produce the processor assignment list for allelements.

PFGEN uses the processor assignment list to produce the partition file used as input to ParaDyn.

Database Development for Parallel Applications and Visualization

The results of an analysis with DYNA3D and NIKE3D are written into binary databases for subsequent visualization with the post-processor, GRIZ. Efficient use of on-line and off-line storage and networks strongly suggests limiting the size of the databases as much as possible for large runs. This is especially true for a dynamic analysis in which animations provide optimal understanding and interpretation of the results.

Mili, a new mesh input/output library, provides a self-describing database that has the desirable feature that the content of the database can be limited by providing templates in the analysis programs. Furthermore, Mili provides cross-platform database portability. This allows targeting of the database for the desired post-processing environment. Requirements for databases generated in a parallel calculation naturally fit into the grid object design provided with the Mili design. The Mili library development for writing the databases has been completed in this last year. The modifications needed in GRIZ for reading the Mili database will be continued into next year along with a parallel implementation for GRIZ.

Future Work

Our future work will focus on three significant activities: (1) message-passing research for NIKE3D; (2) parallel contact algorithms for both NIKE3D and DYNA3D; and (3) parallel visualization.

Linear solver research for NIKE3D is being planned as a collaborative activity with the Center for Applied Science and Engineering at the Lawrence Livermore National Laboratory (LLNL).⁶

Mathematical research is being conducted in both parallel iterative solvers and direct solvers using a message-passing interface (MPI). Improved preconditioning methods are being investigated for iterative solvers and several methods for direct solvers are being designed and written.⁷

We will be designing parallel versions of penalty contact algorithms in DYNA3D that allow the contact surfaces to be partitioned over multiple processors. Lagrangian methods are not conveniently or efficiently treated in this way as coordinate and velocity values at an advanced timestep are required during the calculation of the constraint condition. Parallel techniques developed for contact in DYNA3D provide the experience needed to design parallel contact for NIKE3D.

We will continue to work on the parallel automatic contact algorithm in DYNA3D to incorporate new features such as boxes and multiple automatic contact.

Parallel visualization is essential for the large applications being simulated on the massively parallel computers planned through the Accelerated Strategic Computing Initiative (ASCI) at LLNL. We will be investigating and pursuing client/server models running GRIZ on a small number of processors on the parallel machine and displaying results on an analyst's workstation.

Acknowledgments

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Characterization of Laser-Induced Mechanical Failure Damage of Optical Components

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The goal of this research is to quantify by numerical calculations and discriminating experiments the effects of surface and subsurface defects on damage initiation and growth in high power laser optical components. The defects include absorbing spots (for example, surface particulate contamination) and surface damage regions (for example, microcracks and voids) which are present due to environmental exposure and fabrication processes. The damage initiation process is described in terms of the stress waves and thermal stresses that develop when intense laser radiation is absorbed by foreign material attached to the optical surface, producing rapid local heating and material evaporation and ablation. The failure and damage growth in the optical components is described using the concepts of fracture and continuum mechanics. Understanding the precursor to damage will lead to surface cleanliness and surface finish design requirements.

Introduction

We investigated the cause of mechanical failure of two optical components due to laser radiation: (1) the Beamlet spatial filter lens, and (2) multilayer dielectric coated mirrors.

Spatial Filter Lens

The Beamlet spatial filter catastrophic failure caused \$128,000 damage to the laser and one month of down-time. Experimental evidence indicates that particulate contamination on the lens

surface was the precursor to failure (Fig. 1). For NIF to set cleanliness and surface finish requirements, we must determine the particulate material and size that results in critical damage morphologies after laser irradiation.

Particulate contamination on optics can act as an obscuration in the beam or as a local initiation site for laser damage. An on-going experimental program, initiated in FY-96 and funded by NIF, is looking at damage morphologies on optical surfaces contaminated with particles of well-controlled size and composition. The experimental effort is focusing on three main types of contamination: organic

Figure 1. Schematic of the formation of pits/faults in glass as various types of surface debris explode on the first shot, and the evolution of these pits/faults into propagating cracks with subsequent shots

(for example, skin and fibers), inorganic (for example, glass chips), and metals (for example, Al). The work is examining the growth of the plasma plume and the initiation of damage when the optic is in air, vacuum, and dry nitrogen.

To improve our understanding of damage initiation and growth, a modeling effort, complementing the experimental work, was also initiated in FY-96. The modeling group is a multidisciplinary team with representatives from NF, Physics, Lasers, and Mechanical Engineering. Physics is responsible for formulating theoretical models of the problem with emphasis on plasma physics, laser-matter interaction, and radiation transport. The Lasers Program is using LASNEX to model the laser interaction with surface particulate, plasma formation, and calculation of the magnitude of the surface pressure pulse on the optic. Mechanical Engineering is using DYNA to investigate the optic material response to the surface pressure pulse calculated by LASNEX. Additionally, Mechanical Engineering is using NIKE and TOPAZ to model crack growth due to cyclic thermal-stress loading.

Multilayer Dielectric Coated Mirrors

This work is a continuation of work started in FY-95. The system output fluence and pulse shape of high peak-power laser systems, such as the prototype

Figure 2. Schematic of a nodule defect. A nodule defect is created when a "seed" particulate is deposited on the substrate or thin film layer during the multilayer coating process

Beam Jet Laser and the proposed NF, are influenced by the damage threshold of the multilayer coatings used in the high-power optical components such as mirrors and polarizers. In multilayer dielectric coated mirrors, the predominant surface defects are micron-scale domes associated with the classic nodule defect. These defects are initiated at seed particles that are either present on the substrate, or that are deposited during the film deposition process (Fig. 2). Upon laser illumination, these defects give rise to local electric field enhancements which lead to "hot spots" in the coatings. These rapidly expanding regions create tensile stresses, which may result in mechanical failure of the coatings.

During FY-96, we performed electro-thermal-mechanical modeling of rotationally symmetric nodular defect geometries, assuming normal incidence illumination. We studied the influence of defect geometry (for example, nodule size, depth, and material composition) on the location and magnitude of the "hot spots" and thermal stresses.

Progress

Spatial Filter Lens

Material Dynamic Response. Our effort has focused on using DYNA to model the optic material response to a surface pressure or energy deposition loading calculated by LASNEX. This is not a routine modeling effort, due to the small time scale of the laser pulse (5 ns) and the magnitude of the pressure pulse (15 GPa). Additional calculations have been performed assuming an aluminum particle on the surface of the optic being irradiated by the laser.

A literature review was conducted to find information on the dynamic properties and failure modes of brittle materials, concentrating on SiO₂ and other forms of glass. For brittle materials the mechanical properties vary drastically from virgin material to damaged material. This necessitates a material model that accounts for rate-dependent cumulative damage and associated material property degradation. Many damage models exist for brittle materials, ranging from pure phenomenological models to ones that incorporate damage nucleation and the growth and coalescence of microcracks. At this point it is not clear which model would be best for our particular case. It may require combining certain features of existing models with new features to accurately predict SiO₂ damage based on the results of experiments.

If a metal particle on the front side of an optic is hit with a laser, a pressure pulse due to the laser light absorption on the surface of the particle will be

transmitted through the particle. Spallation of the particle may occur if the particle is not flush against the optics surface. The spallation is due to the crossing of two rarefaction waves, one from the front of the particle when the loading falls off, and the other generated from the rear surface when the incident shock reflects back into the material. If the tensile conditions are sufficient in magnitude and time application, they can lead to the formation of a spall plane. Spallation calculations were performed using a Tuler-Butcher time-dependent failure model to predict the amount of particle debris that may be deposited onto the surface of the SiO_2 from laser illumination on the front surface. A Gaussian full-width half-maximum pressure pulse was applied to one end of a 100- μm long aluminum bar with the other end free. **Figure 3** shows the peak pressure of the Gaussian pulse at various pulse widths required to initiate spallation. The pressure required to cause spallation at pulse widths less than 5 ns increases significantly, indicating the need for a time derivative failure model.

An Al particle on the front surface of the optic was modeled with DYNAST. The Al particle was placed in 20° half-angle contact with a SiO_2 substrate. A 150-kbar, 4-ns Gaussian pressure pulse was applied to the surface of the sphere with a $\cos^2\theta$ pressure distribution. The Steinberg-Guinan constitutive law, Mie-Grueneisen equation of state and the Tuler-Butcher failure criteria for damage were used to model the behavior of the Al particle. The SiO_2 substrate was modeled with an elastic plastic constitutive model and a Mie-Grueneisen equation of state. Failure in the substrate was modeled with a simple spall criterion. Failure in the

Figure 3. Maximum pressure of a Gaussian pulse required to cause spallation in a 1-D plane strain analysis of an Al bar. The pressure required to cause spallation at pulse widths less than 5 ns increases significantly, indicating the need for a time-derivative failure model.

substrate occurs when the maximum principle stress reaches a tensile limit of 6.5 kbar. When failure occurs, the deviatoric stresses are set to zero and the element can only handle compressive pressures. A complete brittle damage model is not used for the SiO_2 at this time, which should account for cumulative damage, time-dependent failure and compressive failure. **Figure 4** shows the cumulated damage in the Al particle and SiO_2 substrate after 50 ns. These calculations begin to address the association of surface contaminants with the initiation of damage sites on the SiO_2 optic.

Crack Growth Dynamics. After the damage starts, the cracks can grow until they reach a detectable size, at which time the optic component is removed from service before it can fail catastrophically. The cracks may grow by a number of mechanisms: (1) thermally-induced crack growth due to time varying stresses; (2) crack growth due to the propagation of stress waves from rapidly heated

Figure 4. Cumulative damage in an Al particle and SiO_2 substrate after 50 ns. Failure in the substrate, using a simple spall criterion, occurs when the maximum principle stress reaches a tensile limit of 6.5 kbar.

defect sites near the surface; and (3) crack growth due to plasma formation in existing surface cracks. The damage from these mechanisms cause both optical and mechanical changes in performance.

For thermally-induced crack growth there are critical length scales relating the size of the absorbing defect, the crack size, and the distance between the hot spot and the crack. Beyond a certain separation of the hot spot and the crack there is not enough energy in the laser pulse to initiate crack growth. This envelope of thermal stress damage has started to be quantified by thermal cracking calculations.

Near the absorbing defect, the optical material experiences large temperature changes that induce large residual stresses and cracking upon cooldown. Thermally-induced crack growth in these regions must depend on the time- and temperature-dependent viscous response of the silica constitutive model. This constitutive model, and the analytical tools to measure the propensity for cracking under such conditions are in the process of development.

In this first series of analyses, the crack is 50 μm beneath the surface and 100 μm in length. The orientation of the crack is parallel to the surface. The laser energy flux of $1.85 \times 10^9 \text{ W/m}^2$ is deposited over a spot size of 75 μm . Figure 5a

Figure 5. Temperature field (a) and stress state (b) near a subsurface crack. The crack acts as a barrier to thermal diffusion, forcing the heat flow around the ends of the crack, and thereby causing thermal gradients and singular stresses

shows the temperature contours near the crack at 2 ms. The crack acts as a barrier to thermal diffusion, forcing the heat flow around the ends of the crack, causing thermal gradients and singular stresses. Figure 5b shows contours of the maximum principal stress concentrating around the crack tips with a pattern characteristic of mixed mode I and II loading. The energy available for crack advance at the crack tip as a result of these loading conditions is 14.0 J/m^2 . This is a very small fraction of the energy absorbed at the surface ($3.7 \times 10^6 \text{ J/m}^2$), but large enough to initiate cracking in the material based on adding the mode I and mode II stress intensity factors. The root mean square addition of the mode I and mode II stress intensity factors may not be the correct method of predicting mixed mode failure, but an experimentally verified criterion for failure of brittle materials under mixed mode loading is not available.

The importance of this flux level is that it represents a critical value for the onset of crack growth. The thermal stresses represent only one part of the total loading on cracks near a laser surface, but a part which may be particularly important combined with the presence of absorbing optical surface contamination.

Multilayer Dielectric Coated Mirrors

The objective of this task was to identify the precursor and characterize the catastrophic delamination of multilayer dielectric coated mirrors under very high laser fluences. We focused our attention on the nodule defect (Fig. 2). A nodule defect is created when a "seed" particulate, which is usually hafnia because the silica evaporates more continuously, is deposited on the substrate or a layer during the multilayer coating process. Subsequent layers then produce a bump in the silica overcoat. The distortion represented by the nodule causes non-uniformities in the electric field that lead to local hot spots.

During FY-96, we performed electro-thermo-mechanical modeling of rotationally symmetric nodular defect geometries, assuming normal incidence illumination.

The electromagnetic code AMOS was used to calculate the E-field enhancement due to the nodule defect. The E-field is enhanced by a factor of 2 to 4 in or near the defect. The thermal energy deposition scales as E^2 . This creates a local hot spot causing compressive stresses within the region and tensile stresses around it. The heat transfer code TOPAZ2D was used to model the thermal effects due to the electromagnetic energy deposition and

NIKE2D was used to predict the resulting thermal stresses. We believe these tensile stresses are what caused the coating failure.

We looked at six nodule defect models representing a range of seed defect sizes and depths of burial (see Fig. 2 and Table 1). Table 1 gives the thermal and mechanical results for the six models. The third geometry gave the highest temperatures and stresses. However, after many computer simulations investigating thermal-stress levels caused by various size and location nodule defects, we have concluded that the stress levels are just too low to be concerned about as a failure mechanism. The analyses showed that geometry differences alone could not be used as a criterion for failure due to thermal stresses.

We also investigated models which included residual stresses and cracks from the manufacturing process. The above models assume that the initial state of the multilayers is stress-free. However, an intrinsic residual stress exists in the multilayers due to the coating process. We were able to calculate the residual stress for a single layer on a substrate, but could not "dial in" the intrinsic stresses for a multilayer. In fact, no one knows the appropriate intrinsic stresses for the multilayers of interest.

The next effort involved putting a 0.4 μm radius crack between the first hafnia and the second silica layers. We used the J-integral method in NIKE2D to calculate the stress intensity factor for delamination. The thermal gradients produced by the reduced conduction across the crack were insufficient by orders of magnitude to produce the critical stress intensity factor for delamination. Only pressure in the crack exceeding 100 MPa is capable of producing stress intensity factors large enough for crack growth. These porous multilayers readily take in water vapor from the air. If one assumes condensation to liquid water and subsequent heating, pressures of the right order of magnitude for crack growth are possible.

The calculated prediction of failure in sub-micron multilayer coatings is a very difficult problem. While the work reported here has not been successful at identifying failure mechanisms, it has at least highlighted some requirements for future modeling activities, including:

- 1) obtaining reliable material properties for thin films of silica and hafnia;
- 2) defining failure criteria for thin films and their interfaces, such as bonds;
- 3) developing methods for putting intrinsic stresses into the layers as initial conditions; and
- 4) developing an ability to model stress due to phase change of materials and trapped water.

Future Work

Our focus for FY-97 will be a continuation of the calculations investigating the spatial filter material response due to stress waves caused by the formation of surface plasma plumes, and calculations investigating crack growth and fracture. We are expecting NIF to continue funding the experimental effort and the LASNEX calculations in FY-97. Continuation of the LASNEX calculations are essential to our effort because they define the boundary condition to be used in DYNA.

The 1-D plane strain calculations supplied an understanding of the stress state in the SiO_2 due to pressure/thermal/energy deposition loading. However, the damage observed in the optics is of a 2-D nature. Two-dimensional and possible 3-D calculations are required to understand and adequately model the observed damage. The merging of the LASNEX and DYNA calculations is required to properly model the vapor-liquid-solid interfaces observed on the surface of the SiO_2 when modeling rear surface particles. An extension of the 2-D modeling will be the incorporation of material failure via one or a combination of several brittle

Table 1. Results from investigation of the six geometries in Fig. 2. Local hot spots resulting from the E-field enhancement due to the nodule defect cause tensile stresses around the defect. The thermal stresses alone are not sufficient to cause failure at NIF operating conditions.

Geometry	d	T	D/2	Seed Material	Tmax (K)	Stress (MPa)
						$[\sigma_{\text{max}}^{\text{prin}} - \sigma_{\text{min}}^{\text{prin}}]_{\text{max}}$
1	0.730	1.9723	1.6969	HfO_2	469.6	25.1
2	0.250	1.9723	0.9931	HfO_2	470.4	36.4
3	1.500	1.9723	2.2205	HfO_2	1000.5	136.0
4	.730	1.0087	1.2135	HfO_2	636.4	58.3
5	.730	2.9359	2.0704	HfO_2	408.3	25.7
6	.730	1.9723	1.6969	SiO_2	576.8	34.9

damage models. Failure in this sense is termed bulk material failure, including microcracking, versus explicitly modeling a crack and calculating propagation rates, which will be addressed separately.

A sizable fraction of failures are associated with crack growth. Crack extension from an existing crack can be predicted based on a critical energy release rate (a J -integral value), which in turn is related to a critical stress intensity factor. A J -integral capability has been implemented for use with NIKE2D and TOPAZ2D. This capability will be implemented in the 3-D codes, NIKE3D and TOPAZ3D. Additionally, the J -integral capabilities will be implemented in the DYNA codes to model

crack propagation resulting from dynamic mechanical events. The J -integral capability will allow us to predict dynamic, static, and thermal loads which would cause crack growth and failure. The J -integral predictive capability will be validated with the NIF-funded experimental effort.

With a better understanding of the physics behind the observed damage, one hopes to be able to develop a predictive capability which can be used to establish critical flaw sizes to prevent catastrophic optics failure. The multidisciplinary team represents a technically potent attempt to solve the laser damage issues, with every facet of the problem represented in the integrated team.

New Rigid Body Features in DYNA3D

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We have implemented two new rigid body features in the explicit finite element code DYNA3D. The first is the modified Rigid Body Joints that provides a tighter bond between rigid bodies with reasonable integration time increments. The second feature is Material Switching, a capability that allows groups of materials to be changed from deformable to rigid then back at user-specified times.

Introduction

As DYNA3D is increasingly applied to analyzing mechanical systems and impact simulations, adding new functionalities involving rigid body mechanics/kinematics becomes more important. One such example is the capability to model joints, such as revolute, universal or spherical joints in complicated machinery or suspension systems. The Rigid Body Joints feature in DYNA3D¹ did provide the necessary modeling tool. However, ideal bonding conditions could only be achieved at the expense of requiring very small integration time steps. This deficiency occurs because the penalty stiffness between adjoining rigid bodies was considered a function of the time step.

A new algorithm based on a rigid body mechanics approach is implemented to overcome this shortcoming. The new method is always stable with the time step, limited by the Courant stability condition, and the bonding force between two adjoining rigid bodies is calculated according to their masses and current distance.

In some impact applications of DYNA3D, "freezing" the entire model or part of the model as a rigid body during a specific period of time appears to have no adverse effect on the overall simulation, but does offer a significant economic advantage. One example is the simulation of multiple ground impacts of an object during a drop test. Depending on the model characteristics, such as the material

properties and model geometry, and the kinematic parameters, such as the drop height, angle and initial velocity, the oscillatory deformation occurring between impacts may be secondary compared to the gross deformation inflicted by ground impacts. Thus, treating the whole or part of the model as a rigid body between impacts could save considerable CPU time.

The other example is a vehicle impacting a roadside safety structure such as a highway guardrail at high speed. In this case, the post-impact vehicle trajectory is of particular interest because of its likely interference with the traffic flow or rollover. Since the overall vehicle motion is far more important than the component deformation in the vehicle redirection stage, it is desirable to have the finite element mesh treated like a rigid body. The new Material Switching feature in DYNA3D allows individual components (material groups) to be switched back and forth between any deformable and rigid material types at user-specified times.

Progress

Rigid Body Joint Algorithm

There are six types of joints, namely spherical, revolute, cylindrical, planar, universal and translational, currently available in DYNA3D. These joints are defined by 1 to 3 pairs of nodes, depending on

the particular relative movement between adjoining rigid bodies permitted by each joint type. Each pair of nodes consists of a node from each adjoining body, and a force between this pair of nodes is calculated every time step to prevent the pair from separating. The direction of the forces imposes constraints on the relative motion between the pairs of nodes, which in turn creates the desirable motion characteristics for each joint type, whereas the magnitude of the force determines whether the adjoining bodies are tied together.

In the original joint algorithm, with maintaining the global stability in mind, the force magnitude is determined by the time step, and reducing the time step is the only means to increase the stiffness associated with the penalty spring. The new algorithm instead takes both the time step and masses of the adjoining rigid bodies into consideration to achieve the desired stability.

Without the presence of a bonding force, a gap between a pair of nodes that defines the Rigid Body Joint will be created during a time step Δt . To close this gap, a penalty spring that will impose sufficient force needs to be added. Let us consider two isolated rigid bodies of mass m_1 and m_2 , respectively. The distances d_1 and d_2 these rigid bodies would be moved over a time span of Δt by a force f can be expressed as

$$d_1 = \iint \frac{f}{m_1} dt^2 = \frac{1}{2} \frac{f}{m_1} \Delta t^2 \quad (1)$$

and

$$d_2 = \iint \frac{f}{m_2} dt^2 = \frac{1}{2} \frac{f}{m_2} \Delta t^2. \quad (2)$$

To find the force necessary to close the gap, d , between a pair of nodes defining the joint, we combine Eq. 1 and Eq. 2 to yield

$$d = d_1 + d_2 = \frac{f \Delta t^2}{2} \left(\frac{1}{m_1} + \frac{1}{m_2} \right), \quad (3)$$

and

$$f = \frac{2m_1 m_2}{(m_1 + m_2) \Delta t^2} (d_1 + d_2). \quad (4)$$

The penalty spring stiffness, K_p , can then be obtained by making $d_1 + d_2 = 1$ in Eq. 4:

$$K_p = \frac{2m_1 m_2}{(m_1 + m_2) \Delta t^2}. \quad (5)$$

If the rigid bodies are completely isolated from the rest of the model, K_p will tie them perfectly. However, that is not the case for most problems. A scale factor that provides users with provision to tune the penalty forces is made available in case forces of greater or less magnitude are needed.

A vehicle suspension system is used to demonstrate the effectiveness of this new algorithm. Figure 1 shows the initial stage of the suspension system going up a ramp. Two simulations, one using the original joint algorithm, the other the new joint algorithm, are made, and the results are shown in Fig. 2 and Fig. 3, respectively. Several parts are modeled as rigid bodies and connected by the Rigid Body Joints. One of the critical joints is the revolute joint, placed between the wheel hub and the spindle, through which the loads are transmitted between the vehicle frame and the wheels. With the backing plate removed, the disjuncting of the wheel hub and the spindle can be clearly seen in Fig. 2. This is a direct consequence of insufficient penalty force to hold the joint in place. The time step needs to be reduced to a small fraction of the calculated time step to generate enough forces to keep the parts together. As shown in Fig. 3, when the new algorithm is used with a

Figure 1. A vehicle suspension system going up a ramp.

default time step, the wheel hub and the spindle remained connected, and the motion of the vehicle frame dictates a realistic wheel position.

Time Stability

From a stability standpoint, the new Rigid Body Joint can be simplified as two masses, m_1 and m_2 , connected by a spring with spring constant K_p . The frequency of such a system, ω , can be expressed as

$$\omega = \sqrt{\frac{(m_1 + m_2)K_p}{m_1 m_2}}, \quad (6)$$

and the stability limit is in turn defined by

$$\Delta t_c = \frac{2}{\omega} = \sqrt{\frac{4m_1 m_2}{(m_1 + m_2)K_p}}. \quad (7)$$

Substituting **Eq. 5** into **Eq. 7** yields

$$\Delta t_c = \sqrt{2} \Delta t \quad (8)$$

which indicates that the current time step Δt is always within the stability limit imposed by the penalty spring.

Deformable/Rigid Material Switching

This feature lets users designate lists of materials as material groups. Upon activation of the Deformable/Rigid Material Switching feature, DYNA3D collects the materials in a group and merges them to form a rigid body for the subsequent calculation. When off-time is reached, this rigid body is disassembled and the constituents are returned to their original material types. The boundary conditions for the collective rigid body are determined by superimposing the boundary conditions on each individual constituent. During the rigid phase, all elements are "frozen," that is, the element

quantities, such as stresses, strains, strain energy, and other history-dependent variables, are kept unchanged, whereas the nodal quantities, such as velocities and displacements, are updated by rigid body mechanics/kinematics.

This approach perfectly represents the element states for structural elements since stresses and strains are measured with respect to the element coordinate system. For continuum elements, because their stresses and strains are expressed in terms of global Cartesian coordinates, keeping them constant during rigid body motion could be incorrect if finite rotation is involved.

To maintain the stresses and strains with respect to the right reference frame for the continuum elements at all times, second-order tensor transformations need to be done at every time step. Making such a time consuming effort for bookkeeping purposes during the rigid phase is uneconomical and does not affect the mechanics in any way. Instead, the code calculates the rigid body's principal axes by solving an eigenvalue problem at the activation time, and incrementally updates them to account for the motion the rigid body is undergoing. The continuum element stresses and strains are then transformed to the right configuration according to the accumulative rotation of these principal axes at the end of the rigid phase.

The economical advantages of this feature are three-fold:

- (1) the burdensome element calculations are bypassed during the rigid phase;
- (2) through careful selection, contact checks can be reduced to a minimum during the rigid phase; and
- (3) greater time steps could be used during the rigid phase since accuracy, not stability, is the deciding factor in selecting a time step for rigid materials.

Figure 2. Final configuration, with backing plate removed, using the original Rigid Body Joints

Figure 3. Final configuration, with backing plate removed, using new Rigid Body Joints

The applications of this feature identified to date include multiple-impact simulation, post-impact trajectory analysis, post-event visualization and partial stress initialization of large models. The simulation of a cylinder with initial velocity impacting into a rail is chosen as an example for this feature. Because of double symmetry, only a quarter of the cylinder is modeled. Though the actual impact between the cylinder and the rail is through the Rigid Wall feature in DYNA3D, a block representing the rail is added for demonstration purposes. **Figure 4** shows the finite element mesh for this model.

Additional details for this model can be found in the DYNA3D Example Problem Manual.² Two runs were made, with the Material Switching feature turned off in run 1 but turned on in run 2. The total simulation time is 15 ms, and the entire model was changed to a rigid body at the halfway point in the second run. As expected, the CPU time for the second run is about 50% of that for the first run. The final deformation, kinetic energy history and momentum history in the impact direction are all almost identical for the two runs, which justifies the use of the Material Switching feature. The final deformation for run 2 is shown in **Fig. 5**.

Figure 4. Finite element mesh for a cylinder hitting a rail.

We also recorded the displacements at node 205, a point at the center of the cylinder and in contact with the rail at the beginning, for both runs in **Fig. 6** to monitor the distance between the cylinder and the rail. It is of interest because it provides estimates of when the subsequent impacts would take place. An agreement with run 1 is essential for run 2 in successfully simulating the subsequent impacts.

When the switching feature is used, the cylinder needs to be returned to its original material types before the next impact takes place. Although the results appear promising, the study is not complete. Because of the high initial velocity, the simulation time is not long enough to let gravity bring the cylinder down for a second impact. A lower initial velocity will be used in our future studies of this problem.

Future Work

Rigid Body Joints

We are undertaking the task of making Breakable Rigid Body Joints. The Federal Highways Administration (FHWA) has requested this capability

Figure 5. Final deformation of a cylinder hitting a rail.

Figure 6. Distance between the center of the cylinder and the rail.

to simulate the disintegration of the vehicle parts in the event of a severe impact. Possible failure criteria for the joints are relative velocity or acceleration between the two adjoining parts.

Deformable/Rigid Material Switching

At this time, contact check can be completely eliminated when the entire model is switched to rigid. For more general cases involving partial model switching, we need to design and implement algorithms to identify the contact interactions between the converted rigid parts during the rigid

phase. One possible way is cross-checking contact definitions and switching material groups at the initialization phase and forging a specific contact definition only if all entities involved are switched to rigid.

In addition to the cylinder impact problem, more quantitative studies are scheduled. Boeing Commercial Aircraft is using this feature along with the Dynamic Relaxation feature in DYNA3D to add initial stress in a large scale model. With the possible interest from FHWA, a car/guardrail angle impact simulation model is being prepared. This ability to predict the post-impact vehicle motion and trajectory will be the focal points for the latter case. This feature can also be used to add the post-impact motion of the container to visual display.

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Implicit Rigid Body Static and Dynamic Analysis with NIKE3D

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In this work, special treatment is given to the rigid body formulation for implicit structural analysis. The inertial contribution to the coupled deformable-rigid body equations is first formulated and implemented in the implicit finite element code NIKE3D. Special treatment is then given to the non-symmetric tangent matrix that results from the linearization of these equations. For static problems, the coupling of the rigid body to the flexible finite elements can cause a large bandwidth. A special equation-reordering technique is used to alleviate this problem.

Introduction

In finite element analysis, the rigid body idealization can be exploited for many different problems, both static and dynamic. The die in a metal-forming problem can often be treated as rigid. This would usually be a statics application. In dynamics, the rigid body assumption can be applied to the stiff sub-systems of flexible structures when only the low frequency response is desired. Examples of this are vibration analysis of transportation containers, suspension systems and space structures.

The rigid body formulation in an implicit finite element setting is different in a number of ways from that in an explicit setting, as would be expected. For example, in an explicit code, attention is paid to the control of the critical time step when penalty methods are used to attach rigid bodies. In an implicit code, the penalty method does not impose such a time step restriction. In an explicit formulation, solution of the equilibrium equations is much simpler than that in the implicit formulation. The solution of the non-linear equations is the primary issue in the implicit formulation.

In this work, the equations of motion for coupled rigid-deformable finite elements are formulated and methods of solution are developed to solve the problems efficiently.

Progress

The rigid body material model has been available in NIKE3D for some time for static problems only. In this implementation, a part is made rigid by specifying

its material to be type 20. The kinematics of this rigid part are then described by three translational and three rotational degrees of freedom. Integration of the incremental rotations as provided by the non-linear solution scheme is made by use of the exponential map.

We used a version of Newmark's method for the integration of the rotation rates in the body frame. In formulating the inertial contribution of the rigid bodies to the finite element equations, it is recognized that the inertial tangent matrix is non-symmetric. This presents a major hurdle in the implementation, since full-scale non-symmetric linear solution techniques are far too costly. No valid symmetrized approximation to the tangent matrix is apparent. Furthermore, it is not clear whether the symmetric stiffness updates made by the BFGS method to a symmetrized approximation of the stiffness matrix can be successful in handling the problem. An incomplete tangent matrix could diminish some of the savings rigid bodies offer by causing additional equilibrium iterations.

We have performed a special decomposition of the global stiffness matrix into symmetric and non-symmetric parts, so that independent factorization is made of the two parts by a symmetric and non-symmetric solver. The method is slightly more expensive (by about 10%) than the symmetric solver, due to additional matrix multiplications, but is worth the effort for the dynamics problems.

The rigid body idealization in implicit finite element analysis is attractive, due to the reduction in the number of degrees of freedom in the problem that results. In explicit codes such as DYNA3D, the main economical advantage is derived from the reduction in constitutive evaluations. In an implicit

code the reduction of constitutive evaluations is helpful, but the main advantage of rigid parts is derived from their potential to reduce the size of the stiffness matrix and the time to factorize it.

Although rigid materials will reduce the number of degrees of freedom of a large part with thousands of degrees of freedom to six, it often causes an extremely large amount of coupling between non-adjacent deformable elements that are attached to the rigid body. At times this causes the rigid bodies to make the problem less efficient. This increased bandwidth is due to the inability of the bandwidth minimizer to handle the large amount of coupling caused by the rigid part. A multiple minimum-degree reorder technique with a sparse direct solver is used in lieu of the bandwidth minimization/skyline solver scheme. It is shown to be unaffected by the large amount of coupling and recovers the efficiency provided by rigid bodies.

Rigid Body Dynamics Formulation

In the coupled deformable-rigid problem, degrees of freedom $\mathbf{X}$ are segregated into those that lie within the flexible mesh $\mathbf{X}_f$ and those that lie on the interface of the rigid body $\mathbf{X}_r$. Furthermore, rigid interface degrees of freedom can be computed from the current center of rotation of the rigid body $\mathbf{X}_o$ and the current rigid body position vector $\mathbf{R}$ such that:

$$\mathbf{X} = \begin{Bmatrix} \mathbf{X}_f \\ \mathbf{X}_r \end{Bmatrix} = \begin{Bmatrix} \mathbf{X}_f \\ \mathbf{X}_o + \mathbf{R} \end{Bmatrix} \quad (1)$$

The finite element nodal forces can be treated similarly:

$$\mathbf{f} = \begin{Bmatrix} \mathbf{f}_f \\ \mathbf{f}_r \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_f^I + \mathbf{f}_f^\sigma \\ \mathbf{f}_r^I + \mathbf{f}_r^\sigma \end{Bmatrix} \quad (2)$$

where $\mathbf{f}^I$ is the inertial contribution. To get the equations of motion using the generalized coordinates, the internal virtual work is computed:

$$\mathbf{f} \cdot \delta \mathbf{X} = \mathbf{f} \cdot \begin{Bmatrix} \delta \mathbf{X}_f \\ \delta \mathbf{X}_o + \mathbf{R} \times \delta \theta \end{Bmatrix} \\ = \mathbf{f}_f \cdot \delta \mathbf{X}_f + \mathbf{f}_r \cdot \delta \mathbf{X}_o + \mathbf{M}_r \cdot \delta \theta \quad (3)$$

where θ is the incremental rotation and $\mathbf{M}_r = \mathbf{f}_r \times \mathbf{R}$ is the moment. The forces and moments, $\mathbf{f}_r$ and $\mathbf{M}_r$, at the rigid body interface are in equilibrium with the body forces and moments, $\mathbf{f}_o$ and $\mathbf{M}_o$, applied at the center of rotation and the rigid body inertia such that:

$$m \ddot{\mathbf{X}}_o - m(\omega \times \mathbf{d} + \omega \times \omega \times \mathbf{d}) = \mathbf{f}_r + \mathbf{f}_o \\ -\mathbf{d} \times m \ddot{\mathbf{X}}_o + \mathbf{I} \dot{\omega} + \omega \times \mathbf{I} \omega = \mathbf{M}_r + \mathbf{M}_o \quad (4)$$

where m is the mass, ω is the rotational velocity, $\mathbf{I}$ is the tensor of moments of inertia, and $\mathbf{d}$ is the distance from the center of rotation to the center of mass of the rigid body.

Currently in NIKE3D, Newmark's method¹ is used to integrate the finite element accelerations. To maintain consistency with the flexible portion of the mesh, Newmark's method is chosen over mistep formulations² to integrate the rigid body translational and rotational accelerations. This version integrates the body frame rotational velocity $\mathbf{W}$ and acceleration $\mathbf{A}$. The body frame coordinates are rotated to the inertial frame via the rotation matrix Λ . By this transformation $\omega = \Lambda \mathbf{W}$. The rotational inertia terms in Eq. 4 are transformed to the body coordinates to accommodate the integration scheme, yielding:

$$m \ddot{\mathbf{X}}_o - m \Lambda (\mathbf{A} \times \mathbf{d}^o + \mathbf{W} \times \mathbf{W} \times \mathbf{d}^o) = \mathbf{f}_r + \mathbf{f}_o \\ -\Lambda \mathbf{d}^o \times m \ddot{\mathbf{X}}_o + \Lambda (\mathbf{J} \mathbf{A} + \mathbf{W} \times \mathbf{J} \mathbf{W}) = \mathbf{M}_r + \mathbf{M}_o \quad (5)$$

The following is Newmark's method modified for integration of the rotation rates:

$$\Lambda_{n+1} = \Lambda_n \exp(\Theta_n) \\ \Theta_n = \Delta t \mathbf{W}_n + (\Delta t)^2 \left[\left(\frac{1}{2} - \beta \right) \mathbf{A}_n + \beta \mathbf{A}_{n+1} \right] \\ \mathbf{W}_{n+1} = \mathbf{W}_n + (\Delta t) \left[\left(\frac{1}{2} - \gamma \right) \mathbf{A}_n + \gamma \mathbf{A}_{n+1} \right] \quad (6)$$

Where $\exp(\square)$ is the exponential map operator. The algorithm given by Eq. 6 is substituted into Eq. 5, and then linearized to get the rigid body contribution of the tangent matrix $\mathbf{k}_{rr}$. As it turns out, the inertial part of this tangent matrix is non-symmetric even when the center of rotation is at the center of mass.

We developed a method to minimize the work in solving the non-symmetric system. In view of Eqs. 1 to 3, the linear system of equations can be segregated as follows:

$$\begin{bmatrix} \mathbf{k}_{ff} & \mathbf{k}_{fr} \\ \mathbf{k}_{fr}^T & \mathbf{k}_{rr} \end{bmatrix} \begin{Bmatrix} \Delta \mathbf{X}_f \\ \Delta \mathbf{X}_r \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_f \\ \mathbf{f}_r \end{Bmatrix} \quad (7)$$

where

$$\Delta \mathbf{X}_r = \begin{Bmatrix} \Delta \mathbf{X}_o \\ \Delta \theta \end{Bmatrix}, \quad \mathbf{f}_r = \begin{Bmatrix} \mathbf{f}_o \\ \mathbf{M}_o \end{Bmatrix}.$$

Matrix condensation is performed on Eq. 7 to yield the uncoupled equations:

$$\left[\mathbf{k}_{rr} - \mathbf{k}_{fr}^T \mathbf{k}_{ff}^{-1} \mathbf{k}_{fr} \right] \Delta \mathbf{X}_r = \left\{ \mathbf{f}_r \right\} - \mathbf{k}_{fr}^T \mathbf{k}_{ff}^{-1} \mathbf{f}_f \quad (8)$$

$$[k_{ff}][\Delta x_f] = f_f - [k_{rf}][\Delta x_r] \quad (9)$$

In this method, the rigid body degrees of freedom are solved first from **Eq. 8** with a non-symmetric solver and substituted into **Eq. 9**. The inverse of k_{ff} never needs to be calculated explicitly. Instead, k_{ff} is factorized and then successive back solves are made to form the Schur complement matrix and right hand side in **Eq. 8**. Typically, k_{rf} is small (especially when compared to k_{ff}) such that **Eq. 8** and **Eq. 9** take roughly 10% to 15% longer than the similar size symmetric linear solve for typical problems.

Rigid Body Dynamics Implementation

Bricks, shells, beams and discrete elements can be treated as rigid by specifying the element material type to be 20 in the NIKE3D³ input deck. NIKE3D calculates the moments of inertia, and by default uses the center of mass as the center of rotation. Alternate moments of inertia and centers of rotation along with rigid body initial velocities can be specified on the material cards. Nodes and facets can also be defined as rigid by specifying the nodal list on the appropriate cards. Rigid bodies can be fastened together by use of connecting penalty springs.

Rigid Body Dynamics Applications

A simple top (**Fig. 1**) is given an initial rotation of 1 rad/s about its axis of symmetry 3 ($I_3 = 4.0$) and along the 1 axis ($I_1 = 5.22$), and allowed to rotate freely. Since this is torqueless motion, the angular

Figure 1. Top shown in body coordinate system 123 and inertial coordinate system xyz.

momentum must remain constant. Due to the axis of symmetry, the top will precess about some preferred axes. Solution of the Euler equations shows that the body frame angular velocity vector will rotate about the symmetry axes at a uniform rate, with a period given by

$$T = \frac{2\pi I_1}{(I_1 - I_3)\omega_3^0} = 26.85 \text{ s} \quad (10)$$

The angular velocities computed by NIKE3D, along with the exact answers, are plotted in **Fig. 2**. The rates ω_1 and ω_2 predicted by NIKE3D are nearly exact, while ω_3 is exact. A more complicated motion results when the top is fixed about its pointy end and is given an initial rotational $\omega_3^0 = 1000 \text{ rad/s}$ with a gravitational force acting through its center of mass, causing a moment about its center of rotation. **Figure 3** shows the x displacement of the center of mass as the top rotates. The high frequency response in **Fig. 3** is due to the top's precession, while the low frequency response is due to nutation.

A potential application for rigid body dynamics is the vibrational response of a transportation container. The FL transportation container (**Fig. 4**) has concentric capped cylinders that are separated by foam. The payload rests on plates welded to the inner cylinder. During transport, the outer canister is tied down by guy wires and is relatively rigid. The inner cylinder is also relatively rigid compared to the foam. The low frequency response is dominated by the behavior of the foam. It is then reasonable to make the two cylinders and the payload rigid.

Figure 2. Body frame rotational velocities for precessing top.

A vibrational base acceleration (Fig. 5) was applied to the cylinder and the response was modeled with NIKE3D, with all flexible elements as one case, and the cylinders and payload rigid as another case.

Figure 3. Plot of x-displacement of the center of mass for top spinning under the influence of gravity in the z direction.

Figure 4. FL shipping container.

This amounts to making 6260 of the 7032 shells rigid. The only shells that are flexible are the plates supporting the payload. The horizontal displacement of the payload is shown for both cases in Fig. 6. The fully

Figure 5. Base acceleration input for NIKE3D model of FL container.

Figure 6. Horizontal displacement of payload in FL container due to base acceleration.

Figure 7. Sheet metal stamping.

Table 1. Results from NIKE3D implementation.

	Avg. equation bandwidth	Avg. # of words in stiffness matrix	Avg. time per factorization	Total run time
Case 1. GPS	260	5.6 million	22.0 s	59 min
Case 2. GPS	330	6.6 million	36.0 s	62 min
Case 3. MMD	N/A	1.8 million	6.1 s	29 min

flexible model on the DEC Alpha 2100 took about 31 h with 0.001-s time steps to model the problem out to 1 s. The rigid model took 18 h to complete.

Equation Reordering

As mentioned, using rigid bodies will reduce the number of degrees of freedom but can cause the equation bandwidth to increase drastically, since all the nodes attached to the rigid body are now coupled. Furthermore, GPS⁴ bandwidth minimization is shown to be ineffective in minimizing the bandwidth with such large amounts of coupling. For statics problems the tangent stiffness matrix is symmetric so the decompositions given by **Eqs. 8 and 9** are not necessary. On the other hand, such a decomposition could reduce the large bandwidth. Instead of doing such a factorization, we used a different reordering scheme, called the multiple minimum degree, or MMD.⁵ In the GPS scheme all the terms in the stiffness matrix are reordered in an attempt to push them toward the diagonal to minimize the matrix profile, and thus the storage. With the MMD scheme, reordering is done to minimize the fill in the factorized stiffness matrix. The MMD method tends to push off diagonal terms to the corners of the stiffness matrix.

Implementation and Application of MMD Reordering

The MMD method is used with the sparse direct solver and is specified by selecting option #3 for solver type.

An example is given where rigid bodies do not provide any efficiency using GPS reordering. The mesh shown in **Fig. 7** is a NIKE3D model of a sheet metal stamping. The upper die is displaced downward, stamping the sheet into the lower die. Both the upper and lower die can be considered rigid. Three different cases were run with NIKE3D: 1) all flexible elements; 2) both dies rigid with GPS reordering; and 3) both dies rigid with MMD reordering. The results are shown in **Table 1**.

In Case 1, all the degrees of freedom are fixed on the bottom die, forcing it to be rigid.

As seen from **Table 1**, the rigid body dies do not provide any savings over an all-flexible model. This is due to the top die's not being fixed and free to displace. Its degrees of freedom are therefore coupled with every node on the face of sheet, due to contact. The bottom die is fixed, representing an essential boundary condition whose degrees of freedom don't appear in the stiffness matrix and therefore don't increase the bandwidth. In an analysis where there are only fixed dies, this problem doesn't appear.

Future Work

Currently, only faceted contact is performed with rigid bodies. Contact that exploits the analytical surfaces typical of rigid bodies would provide smooth contact surface to better represent rolling cylinders or other types of rigid body contact. These smooth surfaces would also facilitate convergence of the non-linear equation solving. In addition, rigid bodies can only be connected using flexible elements such as penalty springs. The Lagrange multiplier method would provide a better solution over the penalty spring method to couple rigid bodies.

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Thermal Evaluation of Pantex Pit Storage

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We are modeling the heat transfer and air flow around weapon pit storage containers in Pantex magazines to predict container temperatures. This thermal-fluid mechanics problem presents a significant computational challenge because it involves transient, 3-D natural convection and thermal radiation around a large number of interacting containers with various heat generation rates. We synthesized a modeling procedure for arrays of pit storage containers, and applied the procedure to simulate a recent Lawrence Livermore National Laboratory (LLNL) experiment involving a group of 20 containers. Our calculated container temperatures compare well with data from the experiment, thus validating the modeling procedure. We performed parameter studies to determine the sensitivity of the convection and radiation heat transfer modes, and also demonstrated how the modeling procedure can be applied to an entire Pantex magazine holding 252 pit storage containers.

Introduction

This report investigates potential pit storage configurations that could be used at the Mason and Hanger Pantex Plant. The study uses data from a thermal test series performed at LLNL that simulated these storage configurations. The heat output values used in the LLNL test series do not represent actual pits, but are rounded numbers that were chosen for convenience to allow parameter excursions.

Pits from dismantled nuclear weapons are currently stored in magazines at the Pantex plant in Amarillo, Texas. The pits generate heat due to natural radioactive decay, and therefore may overheat if not cooled properly. Pits are carefully packaged for both structural integrity and fire safety inside cylindrical containers that are stacked closely together in columns inside the magazines. However, the internal container packaging and the compact storage arrangement also thermally insulates the pits, making the problem of cooling more difficult. It is important to keep weapon pits from overheating for safety and reliability.¹

The Pantex pit storage magazines are passively cooled by natural convection and thermal radiation, subjecting them to the diurnal cycle as well as seasonal temperature variations. Heat generated inside the magazine can exceed several kilowatts, raising the internal magazine temperature well above the ambient outdoor temperature. Natural convection cooling occurs because a draft is created by the heat generated inside the magazine, pulling air in through intake vents near the floor while exhausting air out through a ventilation stack in the roof. Thermal radiative exchange occurs between the containers and the surroundings. A full understanding of the thermal transport characteristics of the magazine is desirable to predict pit temperatures under a variety of conditions.

The goal of this work is to develop a robust modeling procedure for analyzing large arrays of pit storage containers. Full-scale discretization of an entire magazine is not possible, due to the complicated geometry of the array of containers, the complexity of the air flow, and the physical limitations of today's computers. In the past there have been both computational and experimental efforts to

analyze Pantex storage magazines,^{1,2,3} but they did not demonstrate the ability to extrapolate away from the known data envelope.

Here we present a different approach that links together two separate computational methods: a detailed fluid mechanics analysis on a few containers, followed by a lumped-parameter thermal model of an array of containers. With this technique, we are predicting container surface temperatures based on the rate of heat generation inside the container. Detailed documentation of our work is presented in Reference 4. We validated our modeling approach by comparing predicted temperatures with data from a recent experiment (performed at LLNL) in which container temperatures were monitored in a controlled, steady-state environment.² Finally, with some modifications to our model, we demonstrated how an entire Pantex magazine can be analyzed.

Progress

We used the commercial finite-element fluid mechanics program FIDAP⁵ to model the air flow around columns of heated cylindrical containers to obtain natural convection coefficients for the containers. Thermal radiation coupling between containers was calculated using traditional view factor techniques⁶ and a Fortran program written specifically for this project. The convection and radiation data were transformed into resistances and used in lumped-parameter modeling, using the commercial

finite-difference code SINDA,⁷ to calculate storage container temperatures. The lumped-parameter resistance network is shown schematically in **Fig. 1**.

Two problem geometries were analyzed: a group of 20 storage containers inside a tent, and a Pantex magazine. The tent is a sub-set of a magazine storage configuration, in which four columns of storage containers were equipped with mock pits producing internal heat generation, instrumented with thermocouples, and monitored in steady-state tests. We selected a data set (Test Run 5, Reference 2) from that experiment for validation of our computational work. Temperature data from the experiment is plotted in **Fig. 2** along with calculated results for the tent model. These results validate the model because the calculated and measured temperatures agree within the range of the data spread.

To analyze the magazine problem with 252 containers we again chose a group of 20 containers, as in the tent, but made modifications to the model (indicated on **Fig. 1**) that adapted it to the highly insulated magazine geometry. This approach allowed a direct comparison of the magazine results with the validated tent results, shown in **Fig. 3**. As expected, the magazine container temperatures are higher than the tent temperatures because the tent radiates to the building while the magazine is insulated by a thick soil berm.

Fluid Mechanics Analysis

A detailed fluid mechanics analysis of the natural convection around the storage containers was required to obtain heat transfer coefficients for the lumped-parameter thermal model. The container diameter is 0.5 m, and the spacing between neighbors is 0.025 m. This close spacing causes the thermal boundary layers of neighboring containers to overlap, and presents a challenging fluids problem because the Rayleigh Number characterizing the flow regime is on the order of 10^8 . Empirical correlations for cylinders with this compact spacing are not available in the literature because very close spacing yields poor heat transfer and thus is not used in common design practice. We were, however, able to confirm the order of magnitude of our calculated results by using a correlation for a single cylinder.⁸

We used FIDAP, with a turbulence wall model, and a 2-D approximation of the containers to obtain the necessary coefficients. We found that the coefficients decrease slowly with both decreasing heat generation rate and decreased spacing between containers. Although the coefficients are actually a function of position around the cylindrical containers, we extracted only average coefficients from

Figure 1. Schematic of lumped-parameter model.

FIDAP for subsequent use in our lumped-parameter models. To quantify the possible error introduced by our modeling assumptions, we lowered the coefficients by 50%, but found that the container surface temperatures rose by only about 1 °C, as Fig. 2 shows.

Thermal Radiation Analysis

Including thermal radiation in the analysis was found to be extremely important in obtaining correct container temperatures. Without radiation, the calculated surface temperatures were 4 to 6 °C higher than the corresponding experimental data (see Fig. 2). To include radiation, the lumped-parameter network code required radiation resistances. To determine these resistances we formulated and solved the radiosity matrices, which relate heat flux to the fourth power of temperature. View factors for each container in the

array were computed using the crossed-string method and view factor algebra.⁶ A total of 253 radiation resistances resulted from this process.

Two different types of storage containers were used in the tent experiment, so this necessitated the use of two different surface emissivities (0.85 for AT-400A and 0.96 for AL-R8) in the calculations. However, we found only 0.1 °C difference in the calculated temperatures when we changed both emissivities to 1.0. This important result shows that assuming black-body radiation is sufficiently accurate to characterize the radiation exchange and will greatly simplify future calculations.

Lumped-Parameter Model

The lumped-parameter approach uses an electrical resistance network analogy to model the response of a thermally interacting system. In Fig. 1

Figure 2. Parameter study of tent model and comparison with experimental data.

Figure 3. Comparison of tent and magazine model results.

we show the network that includes the array of 20 containers and the surrounding components. Each container is connected by radiation with the other 19 containers, but for clarity these connections are not shown in the figure. The convection coefficients and radiation exchanges within the system were translated into thermal resistances for the SINDA runs. **Table 1** lists the values of heat generation² which were used in both tent and magazine models. **Table 2** lists temperature results for the walls, roof, and floor, as well as temperature boundary conditions used in SINDA.

Determination of the temperature of the hot air flowing up the stack requires a calculation of the air flow rate through the magazine. This involved estimating the mass flow rate through the ventilation stack as a balance between the buoyancy forces, which tend to increase the air velocity; the pressure drops in the stack and intake vents, which tend to reduce the air velocity; and the kinetic energy of the air flowing out through the stack. This calculation was an iterative process that resulted in an air flow rate of 0.17 kg/s or 1.5 m/s. While this air flow rate

is reasonable for the idealized models treated here, it may be sensitive to wind speed and direction and will also depend on the heat load within the magazine.

Future Work

We recommend establishing direct air flow rate measurements in the ventilation stacks at Pantex magazines to create a data base on this parameter for improved accuracy in future modeling efforts.

Performing additional studies with our lumped-parameter model will yield further understanding and confidence in this modeling approach. The next logical steps could include the following additions to the model: an array of more than 20 containers, stratification of the air inside the magazine, and dividing each container into more than one lumped mass.

Using commercial software limited our capabilities in the fluid mechanics computation of convection heat transfer coefficients, but it was the most economical way to proceed within the budget of the project. If a more detailed study of

Table 1. Container heat loads used in lumped-parameter model, taken from Test Run 5, Reference 2.

Cont. #	Load (W)	Cont. #	Load (W)	Cont. #	Load (W)	Cont. #	Load (W)
17	12.0	18	12.0	19	12.0	20	12.0
13	12.0	14	12.0	15	12.0	16	12.0
9	12.0	10	12.0	11	12.0	12	12.0
5	15.0	6	7.5	7	15.0	8	7.5
1	5.5	2	15.0	3	5.5	4	15.0

Table 2. Calculated temperatures of surrounding components and boundary conditions from SINDA.

Component	Tent model	Magazine model	Reduced convection	No radiation
T_{floor}	24.1	25.8	24.5	22.9
T_{walls}	23.3	25.6	23.5	22.9
T_{roof}	24.4	28.7	24.3	28.1
$T_{\text{amb air}} \text{ (BC)}$	22.9	22.9	22.9	22.9
$T_{\text{exhaust air}} \text{ (BC)}$	33.2	33.2	33.2	33.2
$T_{\text{building}} \text{ (BC)}$	22.9	n/a	22.9	22.9

the convection is deemed necessary, we recommend proceeding with an LLNL code such as HYDRA⁹ so that the approach can be customized for this specific application.

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Radiation-Induced Thermal Stresses in High-Power Flashlamps

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Accurate calculations of dynamic stresses in pulsed xenon flashlamps, an important lasing component in high-powered glass lasers, will lead to understanding the mechanisms of failure within flashlamp envelopes. The understanding of failure will, in turn, point to more efficient, higher quality, failure-resistant flashlamps. Dynamic stresses in a flashlamp envelope result from two processes: transient heating of the quartz envelope due to radiative absorption, and the pressure rise of the xenon plasma. These stresses were calculated using the 3-D finite-element analysis codes TOPAZ3D, NIKE3D, and DYNA3D. These calculations build upon previous studies of dynamic stresses in envelopes and suggest a possible mechanism of failure due to an extreme temperature rise on the inside surface during the pulse.

Introduction

Flashlamps are the laser pumping source for the NOVA and NIF lasers at Lawrence Livermore National Laboratory. Failure of flashlamps during operation can mean a catastrophic explosion which would severely damage surrounding laser components (such as the amplifier glass). Understanding the mechanisms of flashlamp failure can prevent explosions while increasing flashlamp efficiency and improving flashlamp design.

There are two types of flashlamp failure. The first type is due to fatigue from normal use. This study focuses on the second kind of failure: one-shot failure due to pulsing the flashlamp at an extremely high energy level. This high energy is known as the "explosion energy," or the energy required to explode a flashlamp. The formula for the explosion energy, E_x , is

$$E_x = 20,000 \cdot l \cdot d \cdot \sqrt{t}$$

where l is the arc length of the flashlamp, d is the diameter, and t is the pulse length¹.

This equation is an empirical relationship dating back to Harold Edgerton (1920), the inventor of flash photography. From the explosion energy, the explosion fraction is defined as:

$$f_x = \frac{E}{E_x}$$

where E is the electrical energy delivered to a flashlamp. The lifetime of a flashlamp has been empirically correlated to a simple function of explosion fraction, so understanding of the single-shot explosion mechanism has implications for flashlamp durability.

While a good empirical relationship for the explosion energy is known, the physical failure mechanism is poorly understood. In this project we performed a detailed radiation/conduction/thermal stress analysis of a typical NOVA flashlamp at several explosion fractions. A number of analytical approaches were used to evaluate the optimum method.

Progress

Analytical Approach

This study is an expansion of research on dynamic stresses in the envelopes of pulsed xenon flashlamps. Erlandson² used TOPAZ2D to calculate the temperature distribution in the flashlamp envelopes. Analytic formulae were used to approximate the dynamic stresses due to the envelope temperature distribution and the xenon pressure rise individually. Since that time, experimental data show that the transmissivity of cerium-doped quartz decreases with increasing temperature. This suggests the possibility that as the envelope heats up, the quartz would absorb more

energy, leading to increased temperature rise, leading to higher absorption. This runaway couple could potentially destroy the lamp.

To investigate this possibility, a detailed coupled analysis using TOPAZ3D and NIKE3D was performed. To check the validity of NIKE3D on such a rapid transient problem, DYNA3D was used to check a single case. If the initial analysis showed that it was warranted, a multiple wavelength band coupled radiation/conduction/thermal stress analysis using TRIM 3D was at the ready, though it proved not to be necessary.

Flashlamp Description and Boundary Conditions

A schematic representation of a NOVA flashlamp is shown in **Fig. 1**. The flashlamp arc length is 112 cm and the inner diameter (or bore diameter) is 1.5 cm. The flashlamp envelope is 2.5 mm thick and made of cerium-doped quartz glass. The cerium doping absorbs UV light in the range 0.25 to 0.35 to prevent the solarization of surrounding laser components. The envelope is filled with xenon gas at a fill pressure of 0.04 MPa (300 Torr). Under normal operating conditions, the electrical energy delivered to a flashlamp is 11.4 kJ for a pulse length of 943 ms, which gives a conservative explosion fraction of 0.19. During the pulse, dynamic stresses in the flashlamp envelopes are caused by the temperature and pressure rise of the xenon plasma and the heat absorption due to UV light within the envelope.

Figure 2 shows the mesh model of the flashlamp envelope. Only a piece of the envelope is modeled, taking advantage of symmetry and the extremely long, thin cylindrical characteristics of the envelope (so that end effects can be ignored for short pulse lengths). The mesh is graded at the inner and outer surfaces to capture steep temperature gradients and pressure distributions.

Figure 1. Schematic of flashlamp.

Conditions within the tube were derived using empirical formulas from Erlandson's earlier study of dynamic stresses, mentioned above. The rise in xenon pressure during the pulse is modeled as a uniform pressure on the inside surface of the envelope. The pressure profile during the pulse rises rapidly during the first 100 ms, reaches a peak at around 250 ms, then trails off gradually. A surface heat flux boundary condition on the inner surface of the tube was used to model the effect of the interaction between the xenon plasma molecules and the envelope as well as the absorption of UV wavelengths below 0.12. At these wavelengths the quartz is effectively opaque.

The profile for the surface heat flux boundary condition is similar to the pressure pulse. Additional UV radiation is absorbed within the envelope, due to the cerium doping. For the initial analysis, a single absorption coefficient independent of temperature was used. This volumetric heat absorption is a function of time and position. From these boundary conditions, temperatures and stresses within the envelope are calculated.

Heat Transfer Results

The temperature distribution of the flashlamp envelope was calculated using the 3-D finite-element heat transfer code TOPAZ3D. At the design explosion fraction of 0.19, the peak temperature is about 1150 K on the inside surface (the initial temperature is assumed to be 300 K), as shown in **Fig. 3**. This temperature rise is primarily due to the surface heat flux, and is concentrated within a thin layer near the surface. The volumetric heat generation due to

Figure 2. Finite-element mesh model of a piece of the flashlamp.

cerium doping results in a moderate temperature rise of about 30 K, distributed throughout the envelope. Though each of the two thermal loads contributes about the same total amount of heat to the envelope, the volumetric heat generation results in negligible additional thermal stress because of the weak gradients and small temperature rises.

This would imply that the cerium doping does not materially contribute to flashlamp failure, and thus a more detailed multiband analysis of cerium absorption was not deemed to be necessary.

Figure 4 shows the peak temperatures for explosion fractions of 0.4 and 0.8. At high explosion fractions, the temperature on the inside surface quickly surpasses 2000 K, the softening point (that is, "melting" point) of quartz glass³.

Dynamic Stress Analysis

Stress distributions of the envelope were calculated using NIKE3D, an implicit 3-D finite-element structural mechanics code. At an explosion fraction of 0.19, hoop stress profiles were plotted **Fig. 5**.

Figure 3. Temperature profiles under normal operation conditions ($f_x = 0.19$).

Figure 4. Temperature profiles on inside surface (where peak temperature occurs) for several explosion fractions

Radial stress profiles were also plotted **Fig. 6**. The radial stress due to thermal and pressure loading is in compression and is about one order of magnitude less than the hoop stress. The hoop stress peaks in compression on the inside surface with a magnitude of 23 MPa at 0.7 ms. This high compressive stress is due to thermal loading.

On the inside surface of the envelope, the pressure load is a significant effect only for the first 0.1 ms of the pulse, pushing the inside surface briefly into tension. After the first millimeter past the inside surface, pressure is the dominant load throughout the pulse, causing maximum tensile stresses of about 8 MPa.

NIKE3D quasi-static analysis was used to calculate the envelope stresses. Because the pulse length is so short, two other numerical methods were used to validate the quasi-static assumption. The same analysis was run using the NIKE3D Newmark integration option, which takes inertial terms into account. The problem was also analyzed with the explicit code DYNA3D, for a fully dynamic analysis. A detailed comparison of the stress profiles showed

Figure 5. Profiles of hoop stress under normal operating conditions ($f_x = 0.19$).

Figure 6. Radial stress profiles under normal operating conditions ($f_x = 0.19$).

close agreement between three methods, validating the quasi-static assumption. Run time for the NIKE3D quasi-static method was by far the lowest, so that method was used for the remainder of the analysis.

Studying the envelope stresses under normal operating conditions does not answer questions about one-shot failure of flashlamps. In fact, these stresses are well below the tensile yield strength of quartz glass of 50 MPa and the compressive yield strength of 1100 MPa³. But even at high explosion fractions, the dynamic stresses do not begin to approach the yield strength of quartz glass.

Figure 7 is a plot of hoop stress profiles at $f_x = 0.8$.

So why do flashlamps fail at high explosion fractions?

This evidence suggests that the most likely mechanism involves phase change due to thermal loading. At high explosion fractions, the temperature on the inside surface of the envelope exceeds the melting point of quartz glass. This suggests a possible scenario for failure. During the pulse, the inside surface is under high compressive stress. The inside surface also melts during the shot, deforming and relieving this compressive stress. Within the first millisecond after the pulse, the inner surface solidifies, locking in its current deformed state and creating

high tensile stress. This tensile stress is of the same order of magnitude as the original compressive stress during the pulse, which exceeds the tensile strength of quartz glass, causing failure.

This suggested scenario would imply that during one-shot failure, the flashlamp actually explodes within the millisecond *after* the pulse rather than during the pulse, which would not be easily detectable.

Future Work

Though the initial theory for one-shot flashlamp failure involving cerium doping was not borne out by the analysis, a very likely mechanism has been suggested by these results. Further data on the softening curve of quartz glass at high temperatures should be incorporated into the model. The analysis should be run out to longer times until the envelope has cooled to well below softening temperature. The tensile stresses frozen into the quartz may then be above failure. This work has also identified that a NIKE3D quasi-static analysis gives the required accuracy, and that a multi-band coupled radiation/conduction/thermal stress analysis is not necessary. This greatly simplifies the analysis, so that a larger range of flashlamp models may be tested to verify the hypothesis.

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Figure 7. Stress profiles at a high explosion fraction ($f_x = 0.8$).

imulation of Turbine Fragment Containment and Mitigation

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Researchers at Lawrence Livermore National Laboratory (LLNL) and the Propulsion Research Engineering Division of the Boeing Commercial Airplane Group have been working to improve understanding of the dynamics of jet engine blade failure (fan blade-off events). The work focuses on simulating a blade-off event and the subsequent blade fragment containment. Favorable comparisons between observed fan blade fragment containment and simulation results were achieved in this study. Clarifications of important fan blade-off issues were made as a result of this modeling. Many improvements to DYNA3D were implemented simultaneously.

Introduction

The latest commercial gas turbine engine designs incorporate advanced material technologies that can lead to fan blade failures through either manufacturing imperfections or in-service deterioration. A fan blade failure can lead to high-velocity fragment generation which has the potential for further engine degradation or even airframe damage. The FAA currently requires that commercial aircraft engines be capable of containing the fan blade fragments. LLNL and the Propulsion Research Engineering Division of Boeing Commercial Airplane Group have established a working partnership to further understand and predict the dynamics of these blade-off events. Thus far the work has focused on simulating a blade-off experiment in a generic high-bypass commercial jet engine. In this event, a single blade was purposely failed at the root. The primary blade failure precipitated the failure of an adjacent fan blade but left the remaining blades essentially intact.

Progress

Previous DYNA3D simulations of the blade-off experiment overestimated the consequences of a single blade removal and predicted the loss of a substantial portion of the fan blade assembly. Areas identified as being responsible for the simulation deficiencies included the accuracy and stability of the DYNA3D constitutive relationships in spinning bodies; the initialization of rotating body force loads;

the engine structural responses to dynamically-induced large unbalanced loads; and the response of the fan blade containment cases to blade release and subsequent debris collisions. The first three areas are addressed in this report. The last area, while treated in this study, will be addressed in a project pending between the FAA, LLNL, Boeing, Pratt-Whitney, and Allied Signal.

During the first half of FY-96, deficiencies in the original engine mesh, obtained from an industry source, were identified and enhancements to DYNA3D were made. The DYNA3D modifications included improvements to the tied shell edge slide surfaces during rigid-body spinning. Automatic contact was expanded to include start/stop time specifications, multiple automatic contact definitions, deletion of failed shell elements and nodes, and specification by materials or domains. Other DYNA3D enhancements included multiple definitions by materials for the applications of translational and rotational body force loads, and velocity damping in the automatic contact Lagrangian penetration option. A DYNA3D feature that writes a stress initialization file after completing a dynamic relaxation phase (to reach an initial equilibrium state) was also added. This feature permits the user to modify problem parameters such as load curves and contact definitions between the dynamic relaxation and transient analysis phases.

More recent tasks to clarify the fan blade-off modeling issues and improve the simulation agreement with the observed blade-off responses are briefly described below.

- 1) DYNA3D's ability to accurately and stably simulate spinning bodies was examined. A simplified shaft and blade assembly, with the same radial dimensions and material properties as the more detailed engine mesh was considered. The eight-blade model was spun for ten revolutions. **Figure 1** shows the constant effective stress at a point in one of the rotating blades as a function of angular blade displacement. The stress deviates only slightly from its theoretical constant value.
- 2) Initialization of body forces due to angular rotation and the impulsive effect of a blade release on the subsequent unbalanced shaft motion were studied. These effects were found to be of second order when compared to either the interaction of the blade fragments and the engine, or

Figure 1. Effective stress in a rotating blade with body force loading.

Figure 2. Initial distribution of effective stresses in rotating blades. DYNA3D's stress initialization accurately captures the circumferentially uniform stress state arising from the initial steady engine operation.

the unbalanced shaft load due to a blade loss. The stress state achieved in the DYNA3D analysis as a result of the steady state operation of the engine is shown in **Fig. 2**. Note, as desired, the rotational body forces produce a circumferentially uniform state of effective stress throughout the blade assembly. The initial radial effective stress state shown in **Fig. 2** is consistent with the state of stress expected in the curved fan blade assembly. Similarly, the radial stresses in the fan blade roots produce internal forces which are in agreement with the expected rotational body forces.

- 3) A simple oscillator mesh (a rotating mass at the end of a truss) was checked for the effects of partial body force initialization and subsequent rotational stability in the transient analysis. This provided information on possible variations in the DYNA3D transient analysis solutions under conditions where the initialized rotational body forces are not compatible with the prescribed initial velocity.
- 4) The engine mesh was checked for correct blade masses as well as for the initial clearances between the aluminum containment case and the fan blade assembly.
- 5) The stability of the DYNA3D solution was examined for variance with the code's chosen time step. This was motivated by the aspect ratio of the shaft shell elements, which in some cases had thicknesses in excess of 1.5 times the largest element length. Results of this check indicated that the current time step algorithm provides an appropriate time step size.
- 6) The prebad due to the Kevlar winding on the aluminum case was simulated with thermal prebading.
- 7) The engine shaft bearing's rigidities were checked to ensure that excessive radial translations were not occurring.
- 8) The initial blade release (via the DYNA3D tie-breaking shell/slideline option) was checked for stability during rotational motion.
- 9) Specific contact surfaces were used as a check on the accuracy of the current automatic contact algorithms. Previous fan blade-off simulations used the DYNA3D automatic contact option to model the interaction of the blade fragments, the following blades, and the containment cases. The use of explicit contact surface definitions proved to be among the most productive improvements in the blade-off simulation study.

Results of the calculation with the pre-defined contact surfaces can be seen in **Fig. 3**, which shows the engine approximately one third of a

Figure 3. Fan blade-off simulation with DYNA3D.

revolution after the initial blade release. The red regions in the blades indicate yielding due to the interactions between the blades, the containment cases, and the released blade fragments. The mesh consisted of 108 materials, 11,814 nodes, 2095 beam elements and 10,923 shell elements. Initial blade release and secondary blade failure sequences were numerically invoked with tied nodal sets using experimentally obtained activation times.

Future Work

This project has set the foundation for the FY-97 FAA project by demonstrating that the basic tools are available for high-confidence blade-off simulations involving commercial aircraft and engine debris. However, enhancements to the current automatic contact algorithms are necessary if fan blade-off simulations are to be effectively performed with DYNA3D. In particular, the shell element algorithms should be made more robust to ensure adequate contact representations. Work on a next generation of material failure algorithms is necessary to further advance current blade-off simulation technology.

Currently, fan blade fragmentation is achieved by the release of tied nodal sets at times specified by test results, and the aluminum containment case failure is based on a simple failure criterion (effective plastic strain). These capabilities should be improved to better represent the physics in a blade-off event. The consequences of off-balance engine loads on the overall aircraft structure, including flight stability, and the ramifications of uncontained engine debris on the engine and critical airframe components are also of interest to the FAA and the aircraft industry. They should be further examined as well.

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THRUST AREA REPORT

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