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TWO-DIMENSIONAL STRESS-INDUCED ADIABATIC FLOW

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Abstract

The TENSOR code provides a numerical solution to the propagation of a stress wave of arbitrary amplitude through a Lagrangian grid in two space dimensions. A detailed description of the code is presented in this report. A Fortran listing of the code is available upon request.

I. Introduction

The purpose of this report is to document the TENSOR code in such a way that present users can understand both its formal basis and its limitations. Hopefully, this understanding will allow the user to suggest consistent and meaningful improvements that relate to his specific area of interest.

The code was originally conceived and written by G. Maenchen and S. Sack,¹ and the techniques used by them to difference the equations of motion and components of strain have been retained. However, since the code was used²⁻⁴ to design and interpret experiments for the Flowshare program and as additional material property data for rock became available,⁵⁻⁷ improvements in both the constitutive relations and material interface routines were found necessary.

The code provides a numerical solution to the propagation of a stress wave of arbitrary amplitude through a Lagrangian grid in two space dimensions. A schematic of the code's operation is shown in Fig. 1.

The conservation equations of continuum mechanics are written in differential form in cylindrical Eulerian coordinates $^*(r, \phi, z)$ assuming axial symmetry (ϕ independence). A Lagrangian coordinate system (k, ϕ, l) is established in the material; this coordinate system moves with the material. In practice this means that the material is zoned into elements whose mass remains constant. The Lagrangian coordinates (k, l) assume discrete values: 0, 1, 2, 3, etc.

The Eulerian equations of motion are transformed into the Lagrangian coordinate system and these transformed equations are differenced. These difference equations now provide a functional relation between the applied stress field and the acceleration ($\ddot{u}^n$ in Fig. 1) of a point in the Lagrangian mesh.

* Cartesian geometry (x, y, z) is an available option in the code. In this geometry, the strain in the y direction is zero.

Fig. 1. Incrementing the radial components.

This acceleration is allowed to act over a small time increment so that the mesh becomes distorted ($u^{n+1/2}$ and r^{n+1} are obtained in Fig. 1). The time increment ($\Delta t^{n+1/2}$) is determined by an independent stability condition involving the zone size, the shock strength, and the material sound speed.

The zone distortion is computed quantitatively in terms of strain changes. These strain changes are related to stress changes through the equation of state. In the equation of state, specified for each material in the mesh, pressure is determined from the current zone compression and internal energy. The shear modulus relates the strain deviators to the stress deviators. After the pressure and stress deviators are calculated, they may be adjusted to include plastic flow and crack formation. Time is increased by $\Delta t^{n+1/2}$ and the cycle is repeated using the new stress and new zone coordinates.

The remainder of this report presents a more complete description of the above cycle. In section II the conservation equations of continuum mechanics are given and reduced to the geometry appropriate to the TENSOR Code. Section III gives the differenced momentum equation. Section IV deals with slip surfaces and boundary

conditions. Section V considers strain calculations. Section VI involves the equation of state, and section VII includes the damping and energy calculations, along with the Δt control. A listing of the code is available upon request.

II. Continuum Mechanics

The integral form of the fundamental equations of continuum mechanics is the basis for obtaining both the differential and discontinuity formulation. In this section we follow the technique used by Keller⁸ which allows the particle velocity (u_i) to be different from the velocity of the surface that defines the volume over which the integral equations are written. This distinction is necessary if the jump conditions are to be obtained from the integral formulations.

The surface velocity (v_i) is defined in the following way: $S(t)$ is the surface of an arbitrary volume $V(t)$, and y_i are Cartesian coordinates ($i = 1, 2, 3$).^{*} If the equation for $S(t)$ is

$$\phi(y_i, t) = 0, \quad (II-1)$$

then at a given time t the unit normal ν_i is given by

$$\nu_i = \frac{\partial \phi}{\partial y_i} \left[\left(\frac{\partial \phi}{\partial y_1} \right)^2 + \left(\frac{\partial \phi}{\partial y_2} \right)^2 + \left(\frac{\partial \phi}{\partial y_3} \right)^2 \right]^{-1/2} = \phi_{y_i} (\phi_{y_j} \phi_{y_j})^{-1/2}. \quad (II-2)$$

From Eq. (II-1) we find:

$$\frac{dy_i}{dt} \phi_{y_j} = -\phi_t \quad \left(-\frac{\partial \phi}{\partial t} = \frac{dy_1}{dt} \frac{\partial \phi}{\partial y_1} + \frac{dy_2}{dt} \frac{\partial \phi}{\partial y_2} + \frac{dy_3}{dt} \frac{\partial \phi}{\partial y_3} \right) \quad (II-3)$$

so that an appropriate definition for the surface velocity is

$$v_i = -\phi_t (\phi_{y_j} \phi_{y_j})^{-1/2} \nu_i. \quad (II-4)$$

Notice that v_i is defined to be normal to the surface.

^{*}In this section subscripts y_i and t mean $\frac{\partial}{\partial y_i}$ and $\frac{\partial}{\partial t}$. Repeated indices are to be summed from 1 to 3 so that

$$\phi_{y_j} \phi_{y_j} = \left(\frac{\partial \phi}{\partial y_1} \right)^2 + \left(\frac{\partial \phi}{\partial y_2} \right)^2 + \left(\frac{\partial \phi}{\partial y_3} \right)^2.$$

If λ_i is the unit normal to the surface that points out of V , we have

$$\lambda_j \nu_j = \pm 1 \text{ (summation convention understood)} \quad (II-5)$$

$$dS_i = dS \lambda_i \quad (II-6)$$

where dS is an element of area S .

The way in which the integral form of the conservation equations is obtained is described in the following sections.

1. MASS

Definitions: ρ is density, M is mass.

$$M(y_i, t) = \int_V \rho dV.$$

$$M(y_i + \Delta y_i, t + \Delta t) = \int_{V'} \rho dV + \Delta t \int_S \rho(u_j - v_j) dS_j.$$

Since

$$\lim_{\Delta t \rightarrow 0} \frac{M(y_i + \Delta y_i, t + \Delta t) - M(y_i, t)}{\Delta t} = 0$$

we find

$$\frac{d}{dt} \int_V \rho dV + \int_S \rho(u_j - v_j) dS_j = 0. \quad (II-7)$$

2. LINEAR MOMENTUM

Definitions: P_i is the momentum vector, f_i is body force per unit mass, T_{ij} is the stress tensor, F_i is the total force acting on the volume.

$$P_i(y_i, t) = \int_V \rho u_i dV, \quad P_i(y_i + \Delta y_i, t + \Delta t) = \int_{V'} \rho u_i dV + \Delta t \int_S \rho u_i (u_j - v_j) dS_j,$$

$$\frac{dP_i}{dt} = \frac{d}{dt} \int_V \rho u_i dV + \int_S \rho u_i (u_j - v_j) dS_j,$$

$$F_i = \int_V \rho f_i dV + \int_S T_{ij} dS_j.$$

Since

$$\frac{dP_i}{dt} = F_i,$$

then

$$\frac{d}{dt} \int_V \rho u_i dV = \int_V \rho f_i dV + \int_S [T_{ij} - \rho u_i (u_j - v_j)] dS_j. \quad (11-8)$$

3. ENERGY

Definitions: q_i is the heat flow vector, K is the total kinetic energy, E is the total internal energy, ϵ is the specific internal energy, Q is the rate that heat is leaving (+) or entering (-) the volume, W is the rate at which work is done by the body and surface forces.

$$K(y_i, t) + E(y_i, t) = \int_V \rho \left(\frac{u_i u_i}{2} + \epsilon \right) dV,$$

$$K(y_i + \Delta y_i, t + \Delta t) + E(y_i + \Delta y_i, t + \Delta t) = \int_{V'} \rho \left(\frac{u_i u_i}{2} + \epsilon \right) dV + \Delta t \int_S \rho \left(\frac{u_i u_i}{2} + \epsilon \right) (u_j - v_j) dS_j,$$

$$\frac{d(K + E)}{dt} = \frac{d}{dt} \int_V \rho \left(\frac{u_i u_i}{2} + \epsilon \right) dV + \int_S \rho \left(\frac{u_i u_i}{2} + \epsilon \right) (u_j - v_j) dS_j,$$

$$Q = \int_S q_j dS_j,$$

$$W = \int_V \rho f_i u_i dV + \int_S u_i T_{ij} dS_j.$$

Since

$$\frac{d(K + E)}{dt} = -Q + W,$$

then

$$\frac{d}{dt} \int_V \rho \left(\frac{u_i u_i}{2} + \epsilon \right) dV = \int_V \rho f_i u_i dV + \int_S [u_i T_{ij} - q_j - \rho \left(\frac{u_i u_i}{2} + \epsilon \right) (u_j - v_j)] dS_j. \quad (11-9)$$

4. ANGULAR MOMENTUM

Definitions: B_i is the angular momentum vector, D_i is the moment vector due to the surface and body forces.

$$B_i(y_i, t) = \int_V \rho (y_{i+1} u_{i+2} - y_{i+2} u_{i+1}) dV \quad (i \text{ is not summed}),$$

$$B_i(y_i + \Delta y_i, t + \Delta t) = \int_{V'} \rho (y_{i+1} u_{i+2} - y_{i+2} u_{i+1}) dV + \Delta t \int_S \rho (y_{i+1} u_{i+2} - y_{i+2} u_{i+1})(u_j - v_j) dS_j,$$

$$\frac{dB_i}{dt} = \frac{d}{dt} \int_V \rho (y_{i+1} u_{i+2} - y_{i+2} u_{i+1}) dV + \int_S \rho (y_{i+1} u_{i+2} - y_{i+2} u_{i+1})(u_j - v_j) dS_j,$$

$$D_i = \int_V \rho (y_{i+1} f_{i+2} - y_{i+2} f_{i+1}) dV + \int_S (y_{i+1} T_{i+2,j} - y_{i+2} T_{i+1,j}) dS_j.$$

Since

$$\frac{dB_i}{dt} = D_i,$$

then

$$\begin{aligned} \frac{d}{dt} \int_V \rho (y_{i+1} u_{i+2} - y_{i+2} u_{i+1}) dV &= \int_V \rho (y_{i+1} f_{i+2} - y_{i+2} f_{i+1}) dV \\ &+ \int_S [y_{i+1} T_{i+2,j} - y_{i+2} T_{i+1,j} - \rho (y_{i+1} u_{i+2} - y_{i+2} u_{i+1})(u_j - v_j)] dS_j \\ &\quad (i \text{ is not summed}). \end{aligned} \quad (II-10)$$

5. ENTROPY

Definitions: $\mathcal{A}$ is the entropy per unit mass, T is temperature. The system is defined by the surface $S(t)$. The change in entropy of the system over an infinitesimal time increment (Δt) is

$$\int_{V'} \rho \mathcal{A} dV - \int_V \rho \mathcal{A} dV.$$

The change in entropy of the local surroundings over the same time increment is

$$\Delta t \int_S \left[\frac{q_j}{T} + \rho \phi (u_j - v_j) \right] dS_j.$$

Since the change of entropy of the universe (system and surroundings) is greater than or equal to zero, then

$$\frac{d}{dt} \int_V \rho \phi dV + \int \left[\frac{q_j}{T} + \rho \phi (u_j - v_j) \right] dS_j \geq 0. \quad (\text{II-11})$$

Equations (II-7) through (II-11) are the integral form of the conservation statements concerning mass, linear momentum, energy, angular momentum and entropy. Notice that no assumption has been made concerning the continuity of any of the functions (ρ , ϵ , T_{ij} , etc.) except the surface function $\phi(y_i, t)$; i.e., v_i has a well defined value at every point on the surface.

The conservation of energy formulation [Eq. (II-9)] is used in the TENSOR code to monitor the total energy in the problem. At selected edits, called for by the user, the code gives (see section VII for the difference equations):

$$K + E = \sum_V \rho \left(\frac{u_i u_i}{2} + \epsilon \right) \Delta V, \quad (\text{II-12})$$

along with

$$\int_t W dt = \sum_t \left(\sum_S u_i T_{ij} \Delta S_j \right) \Delta t \quad (\text{II-13})$$

where S is the surface of the grid. Adding to (II-13) the internal and kinetic energy in the grid at the start of the problem gives the total input energy at the edit time. The difference between this input energy and $K + E$ given by Eq. (II-12) gives the energy "check," a useful indication of how the code is operating. Differences larger than 10% of the total input energy should be resolved.

Implicit in this energy calculation is the adiabatic assumption ($q_i = 0$) and the assumption that $u_i = v_i$, i.e., the surface of the grid moves with the particle velocity. At the present time we do not calculate the work done by the body forces f_i (the first term on the left in Eq. (II-9) is not summed). This work term should be included in the code for long-running problems having body forces in the grid if the energy check is to be meaningful.

6. THE DIFFERENTIAL FORM OF THE CONSERVATION EQUATIONS

The integral formulations [Eqs. (II-7) through (II-11)] can be written in differential form by using the divergence theorem,

$$\int_V (A_j)_{y_j} dV = \int_S A_j dS_j \quad (\text{II-14})$$

and Reynolds transport theorem⁹

$$\frac{d}{dt} \int_V A dV = \int_V A_t dV + \int_S A v_j dS_j. \quad (\text{II-15})$$

The functions A and A_i must be continuous for these theorems to be valid. In this section, continuous functions will be assumed.

When Eq. (II-15) is applied to Eq. (II-7), we find

$$\int_V \rho_t dV + \int_S \rho u_j dS_j = 0.$$

The divergence theorem gives

$$\int_V [\rho_t + (\rho u_j)_{y_j}] dV = 0.$$

If the integrand is continuous, then the differential form of the conservation of mass is

$$\rho_t + (\rho u_j)_{y_j} = 0. \quad (\text{II-16})$$

The Reynolds transport theorem applied to Eq. (II-8) gives

$$\int_V (\rho u_i)_t dV = \int_V \rho f_i dV + \int_S (T_{ij} - \rho u_i u_j) dS_j.$$

The divergence theorem gives

$$\int_V [(\rho u_i)_t - f_i - (T_{ij} - \rho u_i u_j)_{y_j}] dV = 0.$$

Making use of Eq. (II-16) gives

$$\int_V \left\{ \rho \left[(u_i)_t + u_j (u_i)_{y_j} - f_i \right] - (T_{ij})_{y_j} \right\} dV = 0.$$

Therefore, the differential form of the conservation of linear momentum is

$$(u_i)_t + u_j (u_i)_{y_j} = f_i + \rho^{-1} (T_{ij})_{y_j}. \quad (\text{II-17})$$

Notice that in order to write the linear momentum statement in this form, the conservation-of-mass equation had to be used.

Applying the two transformation integrals to Eq. (II-9) gives

$$\left[\rho \left(\frac{u_i u_i}{2} + \epsilon \right) \right]_t = \rho f_i u_i + \left[u_i T_{ij} - q_j - \rho \left(\frac{u_i u_i}{2} + \epsilon \right) u_j \right]_{y_j}.$$

When Eqs. (II-16) and (II-17) are used to simplify the above equation, we find that the differential form of the conservation of energy becomes

$$\rho (\epsilon_t + u_j \epsilon_{y_j}) = T_{ij} (u_i)_{y_j} - (q_j)_{y_j}. \quad (\text{II-18})$$

Equation (II-18) shows how the internal energy changes due to the application of a heat flow vector and a stress-velocity field. Notice that the body forces do not directly influence the internal energy change. Their effect is felt through the changes in the velocity field determined by the linear momentum equation where the body forces are directly involved.

When Eqs. (II-14), (II-15), and (II-16) are applied to Eq. (II-10) (the conservation of angular momentum), we find that

$$\begin{aligned} \rho (y_{i+1} u_{i+2} - y_{i+2} u_{i+1})_t + \rho u_j (y_{i+1} u_{i+2} - y_{i+2} u_{i+1})_{y_j} &= \rho (y_{i+1} f_{i+2} - y_{i+2} f_{i+1}) \\ &+ (y_{i+1} T_{i+2,j} - y_{i+2} T_{i+1,j})_{y_j} \quad (i \text{ is no. summed}). \end{aligned}$$

Since

$$(y_{i+1})_t = u_{i+1}, \quad (y_{i+1} T_{i+2,j})_{y_j} = T_{i+2,i+1} + y_{i+1} (T_{i+2,j})_{y_j}$$

and

$$u_j (y_{i+1} u_{i+2})_{y_j} = u_{i+1} u_{i+2} + y_{i+1} u_j (-2)_{y_j},$$

then the above differential form of the angular momentum equation reduces to

$$\begin{aligned} y_{i+1} \left[(u_{i+2})_t + u_j (u_{i+2})_{y_j} - f_{i+2} - \rho^{-1} (T_{i+2,j})_{y_j} \right] \\ - y_{i+2} \left[(u_{i+1})_t + u_j (u_{i+1})_{y_j} - f_{i+1} - \rho^{-1} (T_{i+2,j})_{y_j} \right] \\ = \rho^{-1} [T_{i+2,i+1} - T_{i+1,i+2}]. \end{aligned}$$

Using Eq. (II-17), the differential form of the conservation of angular momentum reduces to

$$T_{i+2, i+1} = T_{i+1, i+2}.$$

Since the Cartesian coordinate system is arbitrary, it may be rotated $\pi/2$ about the y_1 axis so that T_{13} becomes T_{12} , and T_{31} becomes T_{21} . Therefore, the conservation of angular momentum requires that

$$T_{ij} = T_{ji}; \quad (\text{II-19})$$

i.e., the stress tensor must be symmetric.

When Eqs. (II-14), (II-15), and (II-16) are applied to Eq. (II-11), we find that

$$\rho \epsilon_t + \rho u_j \epsilon_{y_j} + (q_j T^{-1})_{y_j} \geq 0. \quad (\text{II-20})$$

Equations (II-16), (II-17), (II-18), (II-19), and (II-20) are the differential forms of the conservation statements concerning mass, linear momentum, angular momentum, and entropy. The continuity of the functions is required for the differential statements to be valid.

Equations (II-17) (linear momentum) and (II-18) (energy) are the conservation equations that are differenced in the TENSOR code. Mass is conserved implicitly by the Lagrangian coordinate system, i.e., there is no mass transport between zones, so that the zone mass remains constant. A symmetric stress tensor, required by Eq. (II-19), is of course used in the code.

7. THE JUMP CONDITIONS

Fig. 2. The volume separation across S' .

If any of the functions (ρ , ϵ , T_{ij} , etc.) have a discontinuity (jump) across a surface S' , then the differential forms of the conservation equations are not valid across this surface. To obtain the conservation equations (jump conditions) across the surface, we choose a volume V bounded by a surface S that is divided into two parts (V_1 and V_2) by the surface S' . Therefore, from Fig. 2,

$$V = V_1 + V_2,$$

$$S = S_1 + S_2. \quad (\text{II-21})$$

If subscripts 1 and 2 denote the value of the function (ρ , ϵ , T_{ij} , etc.) as S' is approached from V_1 or V_2 , then we have

$$(dS'_i)_1 = - (dS'_i)_2 \quad (\text{since the surface is defined using outward normals})$$

$$(v_i)_1 = (v_i)_2 \quad (\text{the surface velocity is uniquely defined}). \quad (\text{II-22})$$

We now write Eqs. (II-7) through (II-11) for each volume (V , V_1 and V_2), subtract the conservation statements for V_1 and V_2 from that for V , and use Eqs. (II-21) and (II-22) to find the jump conditions across S' .

Equation (II-7) gives

$$\begin{aligned} \frac{d}{dt} \int_V \rho dV + \int_S \rho(u_j - v_j) dS_j - \frac{d}{dt} \int_{V_1} \rho dV - \int_{S_1} \rho(u_j - v_j) dS_j \\ - \int_{(S')_1} \rho(u_j - v_j) dS_j - \frac{d}{dt} \int_{V_2} \rho dV - \int_{S_2} \rho(u_j - v_j) dS_j - \int_{(S')_2} \rho(u_j - v_j) dS_j = 0. \end{aligned}$$

Using Eqs. (II-21) and (II-22), we find that

$$\int_{S'} \left\{ \left[\rho(u_j - v_j) \right]_1 - \left[\rho(u_j - v_j) \right]_2 \right\} d(S_j)_2 = 0.$$

Therefore, the mass jump condition is

$$\rho_1(u_j - v_j)_1 (\lambda_j)_2 = \rho_2(u_j - v_j)_2 (\lambda_j)_2.$$

In the remainder of this section, the unit vector $(\lambda_j)_2$ will define the positive direction on the surface S' . Therefore, the following definitions are appropriate:

$$\lambda_j \equiv (\lambda_j)_2$$

$$\Delta \rho \equiv \rho_1 - \rho_2, \quad \Delta \epsilon \equiv \epsilon_1 - \epsilon_2, \quad \Delta T_{ij} \equiv (T_{ij})_1 - (T_{ij})_2, \text{ etc.}$$

$$U \equiv [v_j - (u_j)_1] \lambda_j. \quad (\text{II-23})$$

Using these definitions, the mass jump condition can be written

$$U \Delta \rho = \rho_2 (\Delta u_j) \lambda_j. \quad (\text{II-24})$$

Following the same procedure for the conservation of linear momentum [Eq. (II-8)] gives

$$[T_{ij} - \rho u_i (u_j - v_j)]_1 \lambda_j = [T_{ij} - \rho u_i (u_j - v_j)]_2 \lambda_j.$$

and using Eqs. (II-23) and (II-24), we find

$$\rho_1 U \Delta u_i = - (\Delta T_{ij}) \lambda_j. \quad (\text{II-25})$$

For the conservation of angular momentum [Eq. (II-10)] we obtain

$$y_{i+1} \left[(\Delta T_{i+2, j}) \lambda_j + \rho_1 U \Delta u_{i+2} \right] - y_{i+2} \left[(\Delta T_{i+1, j}) \lambda_j + \rho_1 U \Delta u_{i+1} \right] = 0 \quad (i \text{ not summed}).$$

Since this equation is satisfied by Eq. (II-25), the jump condition for angular momentum is the same as that for linear momentum. However, since Eq. (II-19) must be satisfied inside both V_1 and V_2 , to be consistent with the defined value a function obtains as S' is approached from V_1 or V_2 , we must have

$$\begin{aligned} (T_{ij})_1 &= (T_{ji})_1, \\ (T_{ij})_2 &= (T_{ji})_2, \\ \Delta T_{ij} &= \Delta T_{ji}. \end{aligned} \quad (\text{II-26})$$

We call Eq. (II-26) the angular momentum jump condition, although it is simply a re-statement of Eq. (II-19) at the surface S' .

The jump conditions for energy and entropy are

$$\rho_1 U \Delta \left(\frac{u_i u_i}{2} + \epsilon \right) = - \lambda_j \Delta (u_i T_{ij} - q_j) \quad (\text{II-27})$$

and

$$\lambda_j \Delta \left(\frac{q_j}{T} \right) - \rho_1 U \Delta s \geq 0. \quad (\text{II-28})$$

8. THE JUMP CONDITIONS USED IN THE TENSOR CODE

Equations (II-24) through (II-28) are the conservation statements that must be satisfied across a surface when any of the functions (ρ , ϵ , T_{ij} , etc.) have a sectional discontinuity at the surface.

In the TENSOR code, two types of interior surface discontinuities are considered. The first type (called a slip surface) uses the appropriately modified jump conditions directly in the code; the second type, which gives the jump conditions across a shock front, are called the Hugoniot conditions. The Hugoniot conditions are used to reduce laboratory measurements of shock velocity and particle velocity on selected samples of material to a form that allows the Hugoniot portion of the equation of state to be developed.

The jump conditions for a slip surface are obtained when $\Delta\rho \neq 0$ and $U = 0$; i.e., the density (material properties) may change at the surface S' ($\Delta\rho \neq 0$). However, the surface moves with the same velocity as the normal component of particle velocity on side 1 ($U = 0$). Equation (II-24) becomes

$$(\Delta u_j) \lambda_j = 0; \quad (\text{II-29})$$

i.e., the normal component of particle velocity at the surface must be continuous. To interpret Eq. (II-25), we assume that the surface S' lies in the y_2, y_3 plane and $\lambda_j = \lambda_1 = 1$. Equation (II-25) becomes

$$\rho_1 U \Delta u_1 = -\Delta T_{11}, \quad (\text{II-30})$$

$$\rho_1 U \Delta u_2 = -\Delta T_{21}, \quad (\text{II-31})$$

$$\rho_1 U \Delta u_3 = -\Delta T_{31}. \quad (\text{II-32})$$

Since $U = 0$, Eq. (II-30), (II-31), and (II-32) are satisfied if the stress at the surface is continuous. However, Eq. (II-29) only prevents a jump in the normal component of velocity ($\Delta u_1 = 0$). Equations (II-31) and (II-32) are satisfied if T_{21} and T_{31} are well defined at the surface so that Δu_2 and Δu_3 need not be zero. In the slip surface calculations, T_{21} and T_{31} are defined as zero at the surface and Equations (II-29) through (II-32) become

$$(u_1)_1 = (u_1)_2 \quad (\text{the normal component of velocity is continuous}), \quad (\text{II-33a})$$

$$(T_{11})_1 = (T_{11})_2 \quad (\text{the normal component of stress is continuous}), \quad (\text{II-33b})$$

$$(T_{21})_1 = (T_{21})_2 = 0 \quad (\text{the shear strain is reflected at the boundary}), \quad (\text{II-33c})$$

$$(T_{31})_1 = (T_{31})_2 = 0 \quad (\text{the shear stress is reflected at the boundary}). \quad (\text{II-33d})$$

We attempt to formally satisfy Eq. (II-33) in the code when an interior grid line is a slip surface.

At the exterior of the grid, two other boundary conditions are available in the code; these boundary conditions allow an exterior grid line to be treated either as a free surface (with a pressure profile option) or a semirigid (reflecting) boundary. The free surface boundary conditions are

$$\rho_1 = 0, \quad (\text{II-34a})$$

$$(T_{ij})_1 = -P(t) \delta_{ij} \quad (\text{if } P(t) = 0, \text{ then a true free surface is obtained}). \quad (\text{II-34b})$$

The rigid-wall boundary conditions are

$$\rho_1 = \rho_2 \quad (\text{II-35a})$$

$$u_1 = \Delta u_1 = 0 \quad (\text{no motion normal to the boundary}) \quad (\text{II-35b})$$

$$\left. \begin{aligned} (T_{21})_1 &= (T_{21})_2 = 0 \\ (T_{31})_1 &= (T_{31})_2 = 0 \end{aligned} \right\} \quad (\text{the shear stress is reflected at the boundary}) \quad (\text{II-35c})$$

$$\quad \quad \quad (\text{II-35d})$$

The Hugoniot conditions are obtained if both U and $\Delta\rho$ are different from zero. When this happens, the discontinuity is called a shock. If we assume that the surface S' lies in the y_2, y_3 plane, $\lambda_i = \lambda_1 = 1$ and $v_j \lambda_j = v_1 > 0$, then Eqs. (II-24) and (II-25) can be written as

$$\rho_2 = \frac{\rho_1 U}{U + \Delta u_1} \quad (\text{II-36})$$

and

$$\Delta T_{11} = -\rho_1 U \Delta u_1, \quad (\text{II-37a})$$

$$\Delta T_{21} = -\rho_1 U \Delta u_2, \quad (\text{II-37b})$$

$$\Delta T_{31} = -\rho_1 U \Delta u_3. \quad (\text{II-37c})$$

Using (II-36) and (II-37a) to solve for U gives

$$(\rho_1 U)^2 = - \frac{\Delta T_{11}}{1/\rho_2 - 1/\rho_1}. \quad (\text{II-38})$$

If $\Delta u_2 = \Delta u_3 = \Delta q_i = 0$, then Eq. (II-27) becomes

$$\Delta \epsilon = \frac{(T_{11})_1 + (T_{11})_2}{2} \left(\frac{1}{\rho_1} - \frac{1}{\rho_2} \right). \quad (\text{II-39})$$

Equations (II-36), (II-37a), and (II-39) are the Hugoniot conditions.* These jump conditions allow the density, the normal component of stress, and the internal energy behind the shock front to be calculated when the shock velocity (v_1), the change in particle velocity across the shock front (Δu_1), and the state of the material in front of the shock $[\rho_1, (T_{11})_1, u_1, \epsilon_1]$ are known.

* The conservation relations for a shock wave, first derived by Rankine and Hugoniot for a fluid, are obtained by substituting $(T_{11})_1 = -P_1$ and $(T_{11})_2 = -P_2$ in Eqs. (II-36), (II-37a), and (II-39).

Equation (II-38) shows that a shock exists only if ΔT_{11} and $\Delta \rho$ exist. Therefore, the discontinuities in (II-37b) and (II-37c) must vanish. In the $T_{11}, 1/\rho$ plane, the line that joins the final shock state with the initial shock state is called the Rayleigh line. The slope of this line is equal to $(\rho_1 U)^2$.

If $\Delta \rho = 0$ and $U \neq 0$, then Eq. (II-36) gives $\Delta u_1 = 0$. Equation (II-37) becomes

$$\Delta T_{11} = 0 \quad (\text{II-40a})$$

$$U = -(\rho_1)^{-1} \frac{\Delta T_{21}}{\Delta u_2} = -(\rho_1)^{-1} \frac{\Delta T_{31}}{\Delta u_3} \quad (\text{II-40b})$$

These equations give the velocity of a surface that propagates with a jump in shear stress. The surface propagates in the y_1 direction, with particle velocity in the y_2, y_3 directions. There is no density change across the surface. A wave propagating with these characteristics is called a shear wave.

To summarize this section, the slip surface, free surface and rigid (reflecting) wall boundary conditions used in the code have been stated [Eqs. (II-33), (II-34), and (II-35)] as special cases of the general jump conditions. The jump conditions across a shock were also obtained [Eqs. (II-36), (II-37a), and (II-39)]. Equations (II-36) and (II-37a) are used to develop the Hugoniot portion of the equation of state. Equation (II-39) is used in the code when the Mie-Grüneisen equation of state (section VI) is used as a material model.

9. CYLINDRICAL POLAR COORDINATES

As noted in section II.6, Eqs. (II-17) (linear momentum) and (II-18) (energy) are the conservation equations that are differenced in the TENSOR code. Since these equations have been written for a Cartesian coordinate system and since cylindrical polar coordinates are used in the code, we need to write the momentum and energy equations for a cylindrical polar coordinate system.

In this section we will generalize these two conservation equations for an arbitrary fixed-point coordinate system by replacing both the operators (derivatives) and the tensor components in the Cartesian coordinate system by operators and tensor components that are suitable for any fixed-point coordinate system appropriate to Euclidean space. (Fixed-point coordinates are often called Eulerian coordinates. Equation (II-49a) defines an Eulerian coordinate system.) We will then specify the coordinate system to be cylindrical polar and obtain the momentum and energy laws in the desired coordinate system.

If the law of transformation between two sets of generalized coordinates $\bar{x}^i$ and x^i is given by¹⁰

$$\bar{x}^i = f^i(x^1, x^2, x^3) \quad (\text{II-41})$$

and the inverse transformation exists, so that

$$x^i = g^i(\bar{x}^1, \bar{x}^2, \bar{x}^3).$$

then the differentials $d\bar{x}^i$ and dx^i are given by the linear transformation

$$d\bar{x}^i = c^i_s dx^s \quad (\text{II-42a})$$

$$dx^i = \gamma^i_s d\bar{x}^s \quad (\text{II-42b})$$

where

$$c^i_s = \frac{\partial \bar{x}^i}{\partial x^s} \quad (\text{II-43a})$$

$$\gamma^i_s = \frac{\partial x^i}{\partial \bar{x}^s} \quad (\text{II-43b})$$

A function $B(x^1, x^2, x^3)$ is a tensor of order n if it has 3^n components and if the components transform like (II-42a) or (II-42b) when the coordinates are transformed from x^i to $\bar{x}^i$. If b^r_{st} are the components of B in the x^i coordinate system, then in order for B to be a tensor (of weight zero) its components $\bar{b}^r_{st}$ in the $\bar{x}^i$ coordinate system must be

$$\bar{b}^r_{st} = c^r_m \gamma^n_s \gamma^p_t b^m_{np} \quad (\text{II-44})$$

If Eq. (II-44) is true, then B is a mixed tensor of order 3 having one contravariant index (r) and two covariant indices (s and t). By definition, upper indices are contravariant and lower indices are covariant. Contravariant indices transform using c^i_m and covariant indices transform using γ^m_i , where m is a dummy index. Equation (II-42a) shows that dx^i is a contravariant tensor of order one (a vector). Also, the velocity u^i defined by

$$u^i = \frac{dx^i}{dt} \quad (\text{II-45})$$

is a contravariant vector.¹¹

The indices of tensor components may be lowered or raised by means of the metric tensor g_{rs} and the associated metric tensor g^{rs} .¹² If the position of a point in space is given by its three Cartesian coordinates (y^1, y^2, y^3) , then the distance between two points having coordinates y^i and $y^i + dy^i$ is given by the invariant

$$(ds)^2 = dy^m dy^m \text{ (summed on } m\text{)}. \quad (\text{II-46})$$

Transformation to a curvilinear coordinate system x^i gives

$$(ds)^2 = g_{rs} dx^r dx^s \quad (\text{II-47})$$

where

$$g_{rs} = \frac{\partial y^m}{\partial x^r} \frac{\partial y^m}{\partial x^s} \text{ (summed on } m \text{)}. \quad (\text{II-48})$$

The tensor g_{rs} is an absolute covariant symmetric tensor of order two, and is called the metric tensor. If we denote by g the determinant $|g_{rs}|$ and by G^{rs} the cofactor of g_{rs} in g , then

$$g^{rs} = \frac{G^{rs}}{g} \quad (\text{II-49})$$

is an absolute contravariant tensor of order two and is called the associated metric tensor. Since the coordinate system is fixed, then both the metric tensor and its associate are functions of x^i only. Therefore,

$$\left. \frac{\partial g}{\partial (\text{time})} \right|_{x^i \text{ fixed}} = 0. \quad (\text{II-49a})$$

Two vectors A^r and A_r related such that

$$\begin{aligned} A_r &= g_{rm} A^m \\ A^r &= g^{rm} A_m \end{aligned} \quad (\text{II-50})$$

are called associated vectors; in fact, they are so intimately related that we allow them to represent the same vector, A^r giving the contravariant components and A_r the covariant components of the vector. The covariant components of the velocity vector [Eq. (II-45)] are $u_i = g_{im} u^m$. The indices of higher order tensors can similarly be changed to give associated tensors, i.e.,

$$A^{r..t}_{..s} = g_{sm} A^{rmt} \quad (\text{II-51})$$

Two rules concerning associated tensors are¹³:

1. In any term where there appears a dummy index, we can raise this index from its lower position and at the same time lower it from its upper position without altering the value of the term, i.e.,

$$A^r_{..s} B_r = A_{rs} B^r.$$

2. If there is a free index in every term of a tensor equation, we obtain an equivalent equation by raising or lowering this free index in every place it occurs, i.e., if

$$A_r = B_{rm} C^m,$$

then

$$A^r = B^r_m C^m = B^{rm} C_m.$$

If the curvilinear coordinate system is orthogonal, then

$$g^{mn} = \frac{1}{g_{mn}} = (h_m)^2 \quad (m = n), \quad (\text{II-52a})^*$$

$$g^{mn} = g_{mn} = 0 \quad (m \neq n). \quad (\text{II-52b})$$

We see from Eq. (II-46) that for a Cartesian coordinate system,

$$g^{mn} = \frac{1}{g_{mn}} = 1 \quad (m = n), \quad (\text{II-53a})$$

$$g^{mn} = g_{mn} = 0. \quad (\text{II-53b})$$

Therefore, Eqs. (II-50) and (II-53) show that the covariant and contravariant components of tensors in a Cartesian coordinate system are equal.

The physical components of a tensor¹⁴ in an orthogonal curvilinear coordinate system are obtained by replacing the curvilinear coordinate system at the point in question with a Cartesian coordinate system. The Cartesian coordinate system is oriented so that it coincides with the tangents of the coordinate curves of the curvilinear system. If subscripts α, β, γ correspond to x^1, x^2, x^3 , and the contravariant and covariant components of a vector are A^r and A_r , then the physical components are

$$A_\alpha = h_1 A_1 = \frac{A^1}{h_1}, \quad A_\beta = h_2 A_2 = \frac{A^2}{h_2}, \quad A_\gamma = h_3 A_3 = \frac{A^3}{h_3}. \quad (\text{II-54})$$

The physical components of a second-order tensor A^{rs} are

$$A_{\alpha\alpha} = h_1^2 A_{11} = \frac{A^{11}}{h_1^2}, \quad A_{\beta\gamma} = h_2 h_3 A_{23} = \frac{A^{23}}{h_2 h_3}, \text{ etc.} \quad (\text{II-55})$$

We see that the h_i are simply the scale factors that allow the physical components to have the dimensions (units) appropriate to a Cartesian coordinate system. Again, Eq. (II-53) shows that the covariant, contravariant and physical components of tensors in a Cartesian coordinate system are equal.

*Some authors use: $g_{mn} = \frac{1}{g^{mn}} = (h_m)^2 \quad (m = n).$

In a cylindrical polar coordinate system (x^i) the law of transformation from a Cartesian coordinate system (y^i) is

$$y^1 = x^1 \cos x^2 \quad y^2 = x^1 \sin x^2 \quad y^3 = x^3 \quad (x^1 = r, x^2 = \phi, x^3 = z).$$

The line element is

$$(ds)^2 = (dx^1)^2 + (x^1)^2 (dx^2)^2 + (dx^3)^2.$$

Therefore, from Eqs. (II-47) and (II-52),

$$\begin{aligned} g_{11} &= 1 & g_{22} &= (x^1)^2 & g_{33} &= 1 \\ h_1 &= 1 & h_2 &= \frac{1}{x^1} & h_3 &= 1 \end{aligned} \quad (\text{II-56})$$

and the physical components of the velocity vector are

$$u_r = u^1 = u_1 \quad u_\phi = ru^2 = \frac{u_2}{r} \quad u_z = u^3 = u_3.$$

The following rules apply when an attempt is made to form new tensors by differentiation of other tensors¹⁵:

Rule 1. If A is an invariant (scalar) and a function of a parameter t , then $\frac{dA}{dt}$ is an invariant.

Rule 2. Differentiation of an invariant by the coordinate variables x^i produces a covariant vector, i.e.,

$$\frac{\partial A}{\partial x^i} = B_i \quad \text{where } B_i \text{ is a covariant vector.} \quad (\text{II-57})$$

Rule 3. If differentiation of a tensor by the coordinate variables x^i is accomplished according to the rules of covariant differentiation, then a new tensor results. This new tensor is one order higher in rank, and the increase in order is obtained in the covariant indices.

If A^r is a contravariant vector, then $A^r_{;s}$ is the covariant derivative of A^r where $A^r_{;s}$ is a mixed tensor of second order and

$$A^r_{;s} = \frac{\partial A^r}{\partial x^s} + \left\{ \begin{matrix} r \\ m \ s \end{matrix} \right\} A^m. \quad (\text{II-58})$$

The covariant derivative of a covariant vector A_r is a double covariant tensor $A_{r;s}$ where

$$A_{r;s} = \frac{\partial A_r}{\partial x^s} - \left\{ \begin{matrix} m \\ r \ s \end{matrix} \right\} A_m. \quad (\text{II-59})$$

The covariant derivative of a double covariant tensor A_{rs} is the triple covariant tensor $A_{rs,i}$ where

$$A_{rs,i} = \frac{\partial A_{rs}}{\partial x^i} - \left\{ \begin{matrix} m \\ r \ i \end{matrix} \right\} A_{ms} - \left\{ \begin{matrix} m \\ s \ i \end{matrix} \right\} A_{rm}. \quad (\text{II-60})$$

The symbol $\left\{ \begin{matrix} k \\ \ell \ i \end{matrix} \right\}$ is called a Christoffel symbol of the second kind.¹⁶ If a new tensor is to be formed from a given tensor of order n by the process of covariant differentiation, then n terms must be added to the coordinate derivative

$$\left(\frac{\partial A_{r\ell...}^{pq...}}{\partial x^i} \right).$$

Therefore,

$$\begin{aligned} A_{r\ell...,i}^{pq...} = & \frac{\partial A_{r\ell...}^{pq...}}{\partial x^i} - \left\{ \begin{matrix} m \\ r \ i \end{matrix} \right\} A_{m\ell...}^{pq...} - \left\{ \begin{matrix} m \\ \ell \ i \end{matrix} \right\} A_{rm...}^{pq...} - \dots \\ & + \left\{ \begin{matrix} p \\ m \ i \end{matrix} \right\} A_{r\ell...}^{mq...} + \left\{ \begin{matrix} q \\ m \ i \end{matrix} \right\} A_{r\ell...}^{pm...} + \dots \end{aligned} \quad (\text{II-61})$$

When these n terms are added to the coordinate derivative, they remove the geometrical peculiarities that the x^i coordinate system has introduced into the coordinate derivative that prevent the derivative from forming a new tensor.

If the curvilinear coordinate system is orthogonal, then the Christoffel symbols become

$$\begin{aligned} \left\{ \begin{matrix} i \\ j \ k \end{matrix} \right\} &= 0 \quad \left\{ \begin{matrix} j \\ i \ i \end{matrix} \right\} = \frac{(h_i)^2}{(h_j)^3} \frac{\partial h_i}{\partial x^j} \quad \left\{ \begin{matrix} i \\ i \ j \end{matrix} \right\} = -\frac{1}{h_i} \frac{\partial h_i}{\partial x^j} \\ \left\{ \begin{matrix} i \\ j \ i \end{matrix} \right\} &= -\frac{1}{h_i} \frac{\partial h_i}{\partial x^j} \quad \left\{ \begin{matrix} i \\ i \ i \end{matrix} \right\} = -\frac{1}{h_i} \frac{\partial h_i}{\partial x^i} \end{aligned} \quad (\text{II-62})$$

where the summation convention has been dropped and i, j , and k are all unequal. Since the Christoffel symbols vanish in a Cartesian coordinate system, the covariant derivative reduces to an ordinary partial derivative with respect to the space variable in the Cartesian coordinate system.

Rule 4. Therefore, when a physical law has been formulated in Cartesian coordinates and the formulation contains partial derivatives with respect to the coordinate variable, the derivatives must be replaced with covariant derivatives if the formulation is to be valid in generalized curvilinear coordinates.

Rule 5. The metric tensor (g_{rs}) and the associated metric tensor (g^{rs}) may be considered as constants for the purpose of covariant differentiation (Ricci's lemma¹⁷). Therefore,

$$g_{rs,t} = g^{rs}_{\dots,t} = 0. \quad (\text{II-63})$$

Also, if

$$F^i = T^{ij}_{\dots,j},$$

then from rule 2 concerning associated tensors and Eqs. (II-50) and (II-63),

$$F_i = T_{i,j}^{\cdot j} = \left(g^{jm} T_{im} \right)_{,j} = g^{jm} T_{im,j}. \quad (\text{II-64})$$

Rule 6. If a covariant vector A_r is a function of time (t) and the coordinate variables x^i then the Lagrangian derivative $\frac{dA_r}{dt}$, defined as

$$\frac{d}{dt} A_r = \frac{\partial A_r}{\partial t} + \frac{\partial A_r}{\partial x^j} u^j \left(u^j = \frac{dx^j}{dt} \right) \quad (\text{II-65})$$

is not a vector. This derivative gives the rate of change of the fixed point (Eulerian) tensor component A_r as seen from a material point in a Lagrangian coordinate system. If this derivative is to be evaluated in an Eulerian coordinate system, the right side of Eq. (II-65) must be used. If it is to be evaluated following a material point in a Lagrangian coordinate system, then the left side is used. It is not a vector (tensor) since it does not include the change with distance of the base vectors that define the Eulerian coordinate system.

Since the Lagrangian derivative is a tensor in a Cartesian coordinate system, if we replace $\partial A_r / \partial x^j$ with $A_{r,j}$ in Eq. (II-65), we obtain a covariant vector. This new covariant vector $\delta A_r / \delta t$ is called the material (intrinsic) derivative of A_r where

$$\frac{\delta A_r}{\delta t} = \frac{\partial A_r}{\partial t} + u^j A_{r,j} = \frac{dA_r}{dt} - \left\{ \begin{matrix} m \\ r \quad j \end{matrix} \right\} A_m u^j. \quad (\text{II-66})$$

Similarly, if A^r is a contravariant vector, then

$$\frac{\delta A^r}{\delta t} = \frac{\partial A^r}{\partial t} + u^j A^r_{\dots,j} = \frac{dA^r}{dt} + \left\{ \begin{matrix} r \\ m \quad j \end{matrix} \right\} A^m u^j. \quad (\text{II-67})$$

Notice that u^j remains contravariant in both (II-66) and (II-67) in order to be consistent with Eq. (II-45).

The material derivative is the sum of a Lagrangian derivative and a term that includes the geometrical peculiarities (the changing base vectors) of the Eulerian coordinate system. When the rate at which the base vectors are changing is properly added to the Lagrangian derivative, a tensor derivative is obtained. Since a particle moving through

space will see not only the Lagrangian derivative of a tensor component but also the changes in the tensor's coordinate system, then a true material derivative results only if the coordinate changes are added to the Lagrangian derivative. This is the role played by the Christoffel symbols.

Finally, according to Ricci's lemma (Rule 5 and Eq. (II-49a)), both the metric tensor and the associated metric tensor may be considered constants for the purpose of material differentiation.

Rule 7. The material derivative and the Lagrangian derivative are identical in a Cartesian coordinate system. Therefore, when a physical law has been formulated in Cartesian coordinates and the formulation contains Lagrangian derivatives, these derivatives must be replaced with material derivatives if the formulation is to be valid in generalized curvilinear coordinates. Equation (II-17) can now be written for a generalized curvilinear coordinate system. The contravariant form of this equation becomes

$$\frac{\delta u^i}{\delta t} = f^i + \rho^{-1} T^{ij}_{,j} \quad (\text{II-68})$$

The covariant form is

$$\frac{\delta u_i}{\delta t} = f_i + \rho^{-1} g^{jm} T_{im,j} \quad (\text{II-69})$$

Since in cylindrical polar coordinates $h_1 = 1$, $h_2 = r^{-1}$, $h_3 = 1$, then Eq. (II-62) can be used to obtain the polar coordinate form of the covariant derivatives in the above equations. If Eqs. (II-54) and (II-55) are then used to change the covariant and contravariant indices to physical components, Eqs. (II-68) and (II-69) become

$$\rho \left(\frac{du_r}{dt} - \frac{u_\phi^2}{r} \right) = \frac{1}{r} \frac{\partial}{\partial r} (r T_{rr}) + \frac{1}{r} \frac{\partial}{\partial \phi} (T_{r\phi}) + \frac{\partial}{\partial z} (T_{rz}) - \frac{T_{\phi\phi}}{r} + \rho f_r \quad (\text{II-70a})$$

$$\rho \left(\frac{du_\phi}{dt} + \frac{u_r u_\phi}{r} \right) = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 T_{\phi r}) + \frac{1}{r} \frac{\partial}{\partial \phi} (T_{\phi\phi}) + \frac{\partial}{\partial z} (T_{\phi z}) + \rho f_\phi \quad (\text{II-70b})$$

$$\rho \frac{du_z}{dt} = \frac{1}{r} \frac{\partial}{\partial r} (r T_{zr}) + \frac{1}{r} \frac{\partial}{\partial \phi} (T_{z\phi}) + \frac{\partial}{\partial z} (T_{zz}) + \rho f_z \quad (\text{II-70c})$$

where the symmetric property of the stress tensor has been used. The Lagrangian derivatives are given by

$$\frac{du_r}{dt} = \frac{\partial u_r}{\partial t} + u_r \frac{\partial u_r}{\partial r} + \frac{u_\phi}{r} \frac{\partial u_r}{\partial \phi} + u_z \frac{\partial u_r}{\partial z} \quad (\text{II-71a})$$

$$\frac{du_\phi}{dt} = \frac{\partial u_\phi}{\partial t} + u_r \frac{\partial u_\phi}{\partial r} + \frac{u_\phi}{r} \frac{\partial u_\phi}{\partial \phi} + u_z \frac{\partial u_\phi}{\partial z} \quad (\text{II-71b})$$

$$\frac{du_z}{dt} = \frac{\partial u_z}{\partial t} + u_r \frac{\partial u_z}{\partial r} + \frac{u_\phi}{r} \frac{\partial u_z}{\partial \phi} + u_z \frac{\partial u_z}{\partial z} \quad (\text{II-71c})$$

Equation (II-70) is simply the form that both (II-68) and (II-69) assume when the physical components of the velocity vector and the stress tensor are used in place of the covariant and contravariant components. If we assume $u_\phi = 0$ and axial symmetry, then Eq. (II-70) becomes

$$\rho \frac{du_r}{dt} = \frac{\partial T_{rr}}{\partial r} + \frac{\partial T_{rz}}{\partial z} + \frac{T_{rr} - T_{\phi\phi}}{r} + \rho f_r \quad (\text{II-72a})$$

$$\rho \frac{du_z}{dt} = \frac{\partial T_{zr}}{\partial r} + \frac{\partial T_{zz}}{\partial z} + \frac{T_{zr}}{r} + \rho f_z \quad (\text{II-72b})$$

$$T_{\phi r} = T_{\phi z} = 0. \quad (\text{II-72c})$$

Equations (II-72a) and (II-72b) are the momentum equations that are differenced in the TENSOR code. Equation (II-72c) is satisfied by setting the $r\phi$ and ϕz components of the stress tensor to zero.

The energy equation (II-18) written for a generalized curvilinear coordinate system becomes

$$\rho \frac{d\epsilon}{dt} = T^{ij} u_{i,j}, \quad (\text{II-73})$$

where we have assumed an adiabatic process ($q^j_{,j} = 0$). Notice that for a scalar, the Lagrangian derivative and the material derivative are the same (II-57). Since the stress tensor is symmetric, then Eq. (II-73) can be rewritten giving

$$\rho \frac{d\epsilon}{dt} = T^{ij} e_{ij}, \quad (\text{II-74})$$

where e_{ij} is the strain rate tensor, defined as¹⁸

$$e_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}). \quad (\text{II-75})$$

The strain rate tensor is a symmetric, double covariant tensor. The physical components of the strain rate tensor in the cylindrical polar coordinate system are

$$\begin{aligned} e_{rr} &= \frac{\partial u_r}{\partial r} e_{\phi\phi} = \frac{1}{r} \frac{\partial u_\phi}{\partial \phi} + \frac{u_r}{r} e_{zz} = \frac{\partial u_z}{\partial z} \\ e_{\phi z} &= \frac{1}{2} \left(\frac{\partial u_\phi}{\partial z} + \frac{1}{r} \frac{\partial u_z}{\partial \phi} \right) e_{rz} = \frac{1}{2} \left(\frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z} \right) \\ e_{r\phi} &= \frac{1}{2} \left(\frac{1}{r} \frac{\partial u_r}{\partial \phi} + \frac{\partial u_\phi}{\partial r} - \frac{u_\phi}{r} \right). \end{aligned} \quad (\text{II-76})$$

If $u_\phi = 0$ and there is axial symmetry, then Eqs. (II-74) and (II-76) become

$$\begin{aligned}
e_{rr} &= \frac{\partial u_r}{\partial r} & e_{\phi\phi} &= \frac{u_r}{r} & e_{zz} &= \frac{\partial u_z}{\partial z} \\
e_{rz} &= \frac{1}{2} \left(\frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z} \right) & e_{\phi z} &= e_{r\phi} = 0
\end{aligned} \tag{II-77}$$

and

$$\rho \frac{d\epsilon}{dt} = T_{rr} e_{rr} + T_{zz} e_{zz} + T_{\phi\phi} e_{\phi\phi} + 2T_{rz} e_{rz}. \tag{II-78}$$

Equations (II-77) and (II-78) are the strain rate and energy equations that are differenced in the code.

The conservation of mass [Eq. (II-16)] can be stated very simply in terms of strain rate components. Equation (II-16) becomes

$$\rho^{-1} \left(\frac{d\rho}{dt} \right) = - (e_{rr} + e_{\phi\phi} + e_{zz}). \tag{II-79}$$

This equation provides a very simple interpretation of the trace of the strain rate matrix in terms of the rate of change of density. In a Lagrangian formulation, volume elements are defined by material points, so that mass is conserved implicitly ($\frac{dm}{dt} = 0$). If V is the volume element so defined, then Eq. (II-79) becomes

$$V^{-1} \frac{dV}{dt} = e_{rr} + e_{\phi\phi} + e_{zz} = \Theta. \tag{II-80}$$

Θ is called the dilatation rate. While volume changes are calculated directly in the code according to the change in the zone coordinates between two consecutive cycles, Eq. (II-80) is used to obtain the deviatoric strain rate formulation (section V).

III. The Differenced Momentum Equation

The equations to be differenced are (II-72a) and (II-72b) of section II. Since the equation-of-state formulation will be based on both mean stress and material strength measurements, we separate the stress tensor into mean stress (P) and deviatoric components.

$$\begin{pmatrix} T_{rr} & 0 & T_{rz} \\ 0 & T_{\phi\phi} & 0 \\ T_{rz} & 0 & T_{zz} \end{pmatrix} = \begin{pmatrix} -P & 0 & 0 \\ 0 & -P & 0 \\ 0 & 0 & -P \end{pmatrix} + \begin{pmatrix} T_r & 0 & T_{rz} \\ 0 & T_\phi & 0 \\ T_{rz} & 0 & T_z \end{pmatrix}$$

where

$$\begin{aligned}
P &= -\frac{1}{3} (T_{rr} + T_{\phi\phi} + T_{zz}), \\
T_{rr} &= -P + T_r,
\end{aligned}$$

$$T_{\phi\phi} = -P + T_{\phi},$$

$$T_{zz} = -P + T_z,$$

$$T_{\phi} = -(T_r + T_z).$$

Then if $u = u_r$ and $v = u_z$, Eqs. (II-72a) and (II-72b) can be written

$$\frac{du}{dt} = -\frac{1}{\rho} \frac{\partial(P - T_r)}{\partial r} + \frac{1}{\rho} \frac{\partial T_{rz}}{\partial z} + \frac{2T_r + T_z}{\rho r} + f_r, \quad (\text{III-1})$$

$$\frac{dv}{dt} = -\frac{1}{\rho} \frac{\partial(P - T_z)}{\partial z} + \frac{1}{\rho} \frac{\partial T_{rz}}{\partial r} + \frac{T_{rz}}{\rho r} + f_z. \quad (\text{III-2})$$

(a)

A Lagrangian coordinate system (k, l) is established in the material (Fig. 3a). These coordinates move with the material, and assume discrete values

$$0, 1, 2, \dots, k-1, k, k+1, \dots, k_{\max},$$

$$0, 1, 2, \dots, l-1, l, l+1, \dots, l_{\max}.$$

This coordinate system divides the material into zones with the mass of each zone remaining constant with time. At zero time each k, l coordinate point has a unique Eulerian coordinate $r_{k,l}^0, z_{k,l}^0$ where the Eulerian coordinates are referred to a fixed point. After n cycles, the Eulerian coordinates of the k, l point are $r_{k,l}^n, z_{k,l}^n$.

Fig. 3a. The Lagrangian coordinate system.

Each stress component (Σ) in Eqs. (III-1) and (III-2) is a scalar function of position (r, z) and time (t) . If the Eulerian coordinates are considered to be a function of k, l and t , then since the Lagrangian coordinates do not change with time,

$$\frac{\partial \Sigma}{\partial k} = \frac{\partial \Sigma}{\partial r} \frac{\partial r}{\partial k} + \frac{\partial \Sigma}{\partial z} \frac{\partial z}{\partial k},$$

$$\frac{\partial \Sigma}{\partial l} = \frac{\partial \Sigma}{\partial r} \frac{\partial r}{\partial l} + \frac{\partial \Sigma}{\partial z} \frac{\partial z}{\partial l}.$$

Solving for $\partial \Sigma / \partial r$ and $\partial \Sigma / \partial z$ gives the Lagrangian form of the Eulerian derivatives

$$\frac{\partial \Sigma}{\partial r} = \frac{1}{J} \left(\frac{\partial \Sigma}{\partial k} \frac{\partial z}{\partial l} - \frac{\partial \Sigma}{\partial l} \frac{\partial z}{\partial k} \right) \quad (\text{III-3})$$

and

$$\frac{\partial \Sigma}{\partial \bar{k}} = -\frac{1}{J} \left(\frac{\partial \Sigma}{\partial \bar{k}} \frac{\partial r}{\partial \bar{\ell}} - \frac{\partial \Sigma}{\partial \bar{\ell}} \frac{\partial r}{\partial \bar{k}} \right), \quad (\text{III-4})$$

where the Jacobian^{*} of the transformation (J) is given by

$$J = \frac{\partial r}{\partial \bar{k}} \frac{\partial z}{\partial \bar{\ell}} - \frac{\partial r}{\partial \bar{\ell}} \frac{\partial z}{\partial \bar{k}}. \quad (\text{III-5})$$

Since J will be interpreted to be the zone area, it is important that Eq. (III-5) be positive. The area of the triangle 123 in Fig. 3b is given by

$$\bar{R}_k \times \bar{R}_\ell = |\bar{R}_k| |\bar{R}_\ell| \sin \theta \bar{e} = 2A \bar{e} \quad (\text{III-6})$$

Fig. 3b. The Lagrangian coordinate system.

where the unit vector $\bar{e}$ is normal to the area. The sense of $\bar{e}$ is obtained from the right-hand rule when $\bar{R}_k$ is rotated into $\bar{R}_\ell$ through the smallest angle possible.

If $\bar{e}_r$ and $\bar{e}_z$ are unit vectors in the r and z directions, then

$$\begin{aligned} \bar{R}_k &= (r_1 - r_2) \bar{e}_r + (z_1 - z_2) \bar{e}_z = \frac{\partial r}{\partial \bar{k}} \bar{e}_r + \frac{\partial z}{\partial \bar{k}} \bar{e}_z, \\ \bar{R}_\ell &= (r_2 - r_3) \bar{e}_r + (z_2 - z_3) \bar{e}_z = \frac{\partial r}{\partial \bar{\ell}} \bar{e}_r + \frac{\partial z}{\partial \bar{\ell}} \bar{e}_z, \\ \bar{R}_k \times \bar{R}_\ell &= \left(\frac{\partial r}{\partial \bar{k}} \frac{\partial z}{\partial \bar{\ell}} - \frac{\partial r}{\partial \bar{\ell}} \frac{\partial z}{\partial \bar{k}} \right) \bar{e}_r \times \bar{e}_z = J \bar{e}_r \times \bar{e}_z. \end{aligned} \quad (\text{III-7})$$

Comparing Eqs. (III-6) and (III-7) shows that since A is positive, then J will be positive if the unit vector obtained from $\bar{k} \times \bar{\ell}$ is the same as that obtained from $\bar{e}_r \times \bar{e}_z$. The code has been written assuming this convention has been satisfied. It must be satisfied when the user specifies the coordinates for his problem.

The numbering system used to specify zone corners (mesh points) is shown in Fig. (3a). As a mnemonic to remember the numbering system, we suggest the following:

- (1) When 1 is established at a k, $\bar{\ell}$ point, then 2 is located at the point k - 1, $\bar{\ell}$.
- (2) The remainder of the numbers 3, 4, ... 9 are rotated around the four zones in the direction obtained by rotating $\bar{k}$ into $\bar{\ell}$.

* One is tempted to write $g = J^2$ and apply the formalism of section II.9 to write derivatives of Lagrangian tensors in the Lagrangian coordinate system. In general, this will not be valid since Eq. (II-49a) is not satisfied; i.e., $\frac{\partial J}{\partial k, \ell}$ is not zero. This is the basic difference between Eulerian and Lagrangian coordinates. Since we are only interested in changes in fixed point (Eulerian) tensor components as seen from a Lagrangian coordinate system, we apply the rules of partial differentiation and turn the crank.

Subscripts are used to indicate the mesh point at which a variable is stored. The cycle number (n) is used as a superscript. This superscript may be regarded as the time variable (Fig. 1). Time is incremented in the following way:

$$\begin{aligned}t^{n+1} &= t^n + \Delta t^{n+1/2}, \\t^{n+1/2} &= t^{n-1/2} + \Delta t^n, \\ \Delta t^n &= \frac{\Delta t^{n+1/2} + \Delta t^{n-1/2}}{2},\end{aligned}\tag{III-8}$$

where $\Delta t^{n+1/2}$ is determined from the stability condition (section VII).

Variables that are defined at mesh points are r , z , Δr , Δz , u , v , du/dt , dv/dt .

Therefore,

$$\begin{aligned}r_g^{n+1} &= r(t^{n+1}, k-1, \ell+1), \\ \Delta r_g^{n+1} &= r_g^{n+1} - r_g^o, \\ (ud)_1^n &= \frac{u_1^{n+1/2} - u_1^{n-1/2}}{\Delta t^n} = \frac{du}{dt}, \\ (vd)_1^n &= \frac{v_1^{n+1/2} - v_1^{n-1/2}}{\Delta t^n} = \frac{dv}{dt}, \text{ etc.}\end{aligned}\tag{III-9}$$

Equation (III-9) is the interpretation of the Lagrangian derivative of an Eulerian tensor component at a material point. [See Eq. (II-65) and discussion in section II.] All remaining variables are defined in the interior of a zone; however, they are stored at exterior points and will be given the exterior number that corresponds to their storage location. Therefore, if the interior variables of

ZONE₈₁₆₇ are stored at 7,

ZONE₁₄₅₆ are stored at 6,

ZONE₂₃₄₁ are stored at 1,

ZONE₉₂₁₈ are stored at 8,

then

$$V_1^n = V(t^n, k-1/2, \ell-1/2) = \frac{3}{\pi} \times \text{zone volume},$$

$$M_1 = \rho_1^o V_1^o = \frac{3}{\pi} \times \text{zone mass},$$

$$P_7^n = P(t^n, k + 1/2, \ell + 1/2),$$

$$T_{r6}^n = T_r(t^n, k + 1/2, \ell - 1/2),$$

$$J_8^n = J(t^n, k - 1/2, \ell + 1/2) = \text{zone area } (2J_8^n \text{ is carried in the code), etc.}$$

If the above variables are known at time t^n and if the acceleration $(ud)_1^n$ and $(vd)_1^n$ of the k, ℓ Lagrangian mesh point can be expressed in terms of these variables, then Eq. (III-9) can be used to obtain the velocity at $t^{n+1/2}$ of the k, ℓ point. In the remainder of this section if the superscript is omitted, it is understood to be n .

We consider first the nonderivative terms $(2T_r + T_z)/\rho r$ and $T_{rz}/\rho r$ in Eqs. (III-1) and (III-2). These terms are not affected by the coordinate transformations (III-3) and (III-4). Also, since the stress in each zone is regarded as an interior variable, these nonderivative terms are regarded as an interior acceleration. If the Theorem of Pappus is used to define an average radius in a zone, then

$$\bar{r}_{k+1/2, \ell+1/2} = \frac{V_7}{6J_7}$$

and

$$(\rho r)_{k+1/2, \ell+1/2} = \frac{M_7}{6J_7}.$$

The interior accelerations associated with zone 8167 are

$$\ddot{u}_7 = \frac{6J_7}{M_7} (2T_r + 2Q_r^{n-1/2} + T_z + Q_z^{n-1/2})_7 \quad (\text{III-10})$$

$$\ddot{v}_7 = \frac{6J_7}{M_7} (T_{rz} + Q_{rz}^{n-1/2})_7 \quad (\text{III-11})$$

The Q terms in the above expression are introduced to obtain solutions consistent with both the continuous variable assumption required to obtain the differential form of the conservation equations and the inherent wavelength filtering required by the zoning process. These Q terms are divided into isotropic and deviatoric components where the isotropic component is similar to the artificial viscosity of Von Neumann and Richtmyer.¹ The form that these damping terms take in the code is given in section VII.

The derivative terms are obtained by operating on Eqs. (III-1) and (III-2) with the coordinate transformation defined by Eqs. (III-3) and (III-4). Derivatives in the k and ℓ directions are grouped separately and interpreted to be acceleration components across the 81 and 14 lines for k and across the 12 and 61 lines for ℓ . Therefore,

$$\ddot{u}_{81} = \frac{-2}{(\rho J)_7 + (\rho J)_8} \left[\frac{\partial(P - T_r)}{\partial t} \frac{\partial z}{\partial \ell} + \frac{\partial T_{rz}}{\partial k} \frac{\partial r}{\partial \ell} \right],$$

$$\ddot{u}_{61} = \frac{2}{(\rho J)_7 + (\rho J)_6} \left[\frac{\partial(P - T_r)}{\partial t} \frac{\partial z}{\partial k} + \frac{\partial T_{rz}}{\partial \ell} \frac{\partial r}{\partial k} \right],$$

$$\dot{v}_{81} = \frac{2}{(\rho J)_7 + (\rho J)_8} \left[\frac{\partial(P - T_z)}{\partial k} \frac{\partial r}{\partial \ell} + \frac{\partial T_{rz}}{\partial k} \frac{\partial z}{\partial \ell} \right],$$

$$\dot{v}_{61} = \frac{-2}{(\rho J)_7 + (\rho J)_6} \left[\frac{\partial(P - T_z)}{\partial \ell} \frac{\partial r}{\partial k} + \frac{\partial T_{rz}}{\partial \ell} \frac{\partial z}{\partial k} \right].$$

If

$$\bar{r}_{81} = 2 \left(\frac{\partial r}{\partial \ell} \right) \equiv r_8 - r_1 + \frac{r_7 - r_6 + r_9 - r_2}{2}$$

and

$$\bar{r}_{61} = 2 \left(\frac{\partial r}{\partial k} \right) \equiv r_6 - r_1 + \frac{r_7 - r_8 + r_5 - r_4}{2}$$

along with similar definitions for $\bar{z}_{81}$ and $\bar{z}_{61}$, then the above equations become^{*}

$$\ddot{u}_{61} = \frac{[(P + Q - T_r - Q_r)_7 - (P + Q - T_r - Q_r)_6] \bar{z}_{61} + [(T_{rz} + Q_{rz})_7 - (T_{rz} + Q_{rz})_6] \bar{r}_{61}}{M_7 J_7 / V_7 + M_6 J_6 / V_6}, \quad (\text{III-12})$$

$$\dot{v}_{61} = - \frac{[(P + Q - T_z - Q_z)_7 - (P + Q - T_z - Q_z)_6] \bar{r}_{61} + [(T_{rz} + Q_{rz})_7 - (T_{rz} + Q_{rz})_6] \bar{z}_{61}}{M_7 J_7 / V_7 + M_8 J_8 / V_8}, \quad (\text{III-13})$$

$$\ddot{u}_{81} = - \frac{[(P + Q - T_z - Q_z)_7 - (P + Q - T_z - Q_z)_8] \bar{z}_{81} + [(T_{rz} + Q_{rz})_7 - (T_{rz} + Q_{rz})_8] \bar{r}_{81}}{M_7 J_7 / V_7 + M_8 J_8 / V_8}, \quad (\text{III-14})$$

$$\dot{v}_{81} = \frac{[(P + Q - T_z - Q_z)_7 - (P + Q - T_z - Q_z)_8] \bar{r}_{81} + [(T_{rz} + Q_{rz})_7 - (T_{rz} + Q_{rz})_8] \bar{z}_{81}}{M_7 J_7 / V_7 + M_8 J_8 / V_8}, \quad (\text{III-15})$$

The above 61 components of acceleration are assumed located at $\ell, k + 1/2$ while the 81 components are at $k, \ell + 1/2$. Similar expressions could be written for $\ddot{u}_{12}$ and $\dot{v}_{12}$ ($k - 1/2, \ell$) $\ddot{u}_{14}$ and $\dot{v}_{14}$ ($k, \ell - 1/2$). However, when 1 was located at $k - 1, \ell$, the $\ddot{u}_{12}$ and $\dot{v}_{12}$ components required at k, ℓ were calculated as $\ddot{u}_{61}$ and $\dot{v}_{61}$. Therefore,

*The Q terms in Eqs. (III-12) through (III-15) are centered at $n - 1/2$.

$$(\dot{u}_{61}, \dot{v}_{61})_{k-1, \ell} = (\dot{u}_{12}, \dot{v}_{12})_{k, \ell}$$

$$(\dot{u}_{81}, \dot{v}_{81})_{k, \ell-1} = (\dot{u}_{14}, \dot{v}_{14})_{k, \ell}$$

Also

$$(\ddot{u}_7, \ddot{v}_7)_{k, \ell-1} = (\ddot{u}_6, \ddot{v}_6)_{k, \ell}$$

$$(\ddot{u}_7, \ddot{v}_7)_{k-1, \ell-1} = (\ddot{u}_1, \ddot{v}_1)_{k, \ell}$$

$$(\ddot{u}_7, \ddot{v}_7)_{k-1, \ell} = (\ddot{u}_8, \ddot{v}_8)_{k, \ell}$$

These sixteen acceleration terms (eight for the r component of acceleration and eight for the z component of acceleration) are combined (weighted) to give the acceleration of the k, ℓ point $[(u\dot{d})_1, \text{ and } (v\dot{d})_1]$. The weighting is based on the location of the acceleration terms with respect to the k, ℓ point. The closer the acceleration term to k, ℓ the more influence it has on $(u\dot{d})_1$, and $(v\dot{d})_1$.

Table 1. Acceleration component weight factors.

Acceleration Term	Weight
$\ddot{u}_7, \ddot{v}_7$	$(1 - E_{61})(1 - E_{81})$
$\ddot{u}_8, \ddot{v}_8$	$E_{61} (1 - E_{81})$
$\ddot{u}_1, \ddot{v}_1$	$E_{61} E_{81}$
$\ddot{u}_6, \ddot{v}_6$	$(1 - E_{61}) E_{81}$
$\ddot{u}_{61}, \ddot{v}_{61}$	$(1 - E_{61})$
$\ddot{u}_{81}, \ddot{v}_{81}$	$(1 - E_{81})$
$\ddot{u}_{12}, \ddot{v}_{12}$	E_{61}
$\ddot{u}_{14}, \ddot{v}_{14}$	E_{81}

The weighting factors are E_{61} and E_{81} , where

$$E_{61} = \frac{\bar{R}_{62} \cdot \bar{R}_{61}}{\bar{R}_{62} \cdot \bar{R}_{62}} = \frac{\bar{r}_{62} \bar{r}_{61} + \bar{z}_{62} \bar{z}_{61}}{(\bar{r}_{62})^2 + (\bar{z}_{62})^2}$$

$$E_{81} = \frac{\bar{R}_{84} \cdot \bar{R}_{81}}{\bar{R}_{84} \cdot \bar{R}_{84}} = \frac{\bar{r}_{84} \bar{r}_{81} + \bar{z}_{84} \bar{z}_{81}}{(\bar{r}_{84})^2 + (\bar{z}_{84})^2}$$

The weighting factor for $\ddot{u}_{81}$ is $1 - E_{81}$ while E_{61} is the weight of $\ddot{u}_{12}$. Since the nonderivative terms are interior terms, they are weighted with E_{61} and E_{81} combinations, i.e., $(1 - E_{81})(1 - E_{61})$ is the weight of $\ddot{u}_7$. Table 1 gives the weight factors associated with each acceleration

component. Multiplying the acceleration term by its corresponding weight factor and adding gives

$$(u\dot{d})_1 = [(\ddot{u}_1 - \ddot{u}_6 + \ddot{u}_7 - \ddot{u}_8) E_{61} + \ddot{u}_6 - \ddot{u}_7 + \ddot{u}_{14} - \ddot{u}_{81}] E_{81} \\ + (\ddot{u}_{12} - \ddot{u}_{61} + \ddot{u}_8 - \ddot{u}_7) E_{61} + \ddot{u}_7 + \ddot{u}_{81} + \ddot{u}_{61} + f_r + QKL_r, \quad (\text{III-16})$$

$$(v\dot{d})_1 = [(\ddot{v}_1 - \ddot{v}_6 + \ddot{v}_7 - \ddot{v}_8) E_{61} + \ddot{v}_6 - \ddot{v}_7 + \ddot{v}_{14} - \ddot{v}_{81}] E_{81} \\ + (\ddot{v}_{12} - \ddot{v}_{61} + \ddot{v}_8 - \ddot{v}_7) E_{61} + \ddot{v}_7 + \ddot{v}_{81} + \ddot{v}_{61} + f_z + QKL_z. \quad (\text{III-17})$$

The QKL_r and QKL_z are damping terms used to prevent a special type of zone deformation (section VII).

The velocity of the k, l point is calculated using Eq. (III-9).

$$\begin{aligned} u^{n+1/2} &= u^{n-1/2} + \Delta t^n (u_d)_1, \\ v^{n+1/2} &= v^{n-1/2} + \Delta t^n (v_d)_1. \end{aligned} \quad (\text{II-18})$$

Equations (III-10) through (III-16) give the momentum-differencing scheme used at an interior grid point. These equations allow a new velocity to be calculated at the grid point when the coordinates, stress tensor and density of the four surrounding zones, along with the old grid point velocity, are known. The modification of these equations at an exterior grid boundary (free surface and "rigid" wall) and at an interior grid boundary (slip surface) will now be given.

IV. Boundary Conditions

The formulation of the boundary conditions are given by Eqs. (II-33), (II-34), and (II-35) of section II. We consider each case separately.

1. FREE SURFACE

The free-surface boundary conditions Eq. (II-34), section II require that the density vanish at the boundary and that the stress tensor either vanish or be a specified time-dependent pressure. If $k = 0$ is a free surface, then in Eqs. (III-14) and (III-15),

$$\begin{aligned} M_8/V_8 &= (T_{rz} + Q_{rz})_8 = 0, \\ (P + Q - T_r - Q_r)_8 &= (P + Q - T_z - Q_z)_8 = P_8(t^n), \\ \bar{r}_{81} &= r_8 - r_1 + r_7 - r_6, \\ \bar{z}_{81} &= z_8 - z_1 + z_7 - z_6, \end{aligned}$$

where $P_8(t^n)$ is the specified pressure on $k = 0$ at time t^n . If $P_8(t^n) = 0$, then a true free surface results. The effects of $\dot{u}_1, \dot{v}_1, \dot{u}_8, \dot{v}_8, \dot{u}_{12},$ and $\dot{v}_{12}$ on the acceleration of the k, l point are removed by setting $E_{61} = 0$ in Eqs. (III-16) and (III-17) (Table 1). These five modifications are consistent with replacing the zone 9218 with a zone that extends to infinity in the minus k direction having zero density and a specified pressure.

Table 2 gives the required modifications to Eqs. (III-12) through (III-17) for the exterior free-surface boundary conditions.

Table 2. Free surface boundary conditions.

Boundary	Modifications
k zero	$E_{61} = \frac{M_8}{V_8} = 0$ $\bar{r}_{81} = r_8 - r_1 + r_7 - r_6$ $\bar{z}_{81} = z_8 - z_1 + z_7 - z_6$ $(T_{ij})_8 = -P_8 \delta_{ij}$
k max	$\frac{M_7}{V_7} = 0, E_{61} = 1$ $\bar{r}_{81} = r_8 - r_1 + r_9 - r_2$ $\bar{z}_{81} = z_8 - z_1 + z_9 - z_2$ $(T_{ij})_7 = -P_7 \delta_{ij}$
l zero	$E_{81} = \frac{M_6}{V_6} = 0$ $\bar{r}_{61} = r_{61} + r_{78}$ $\bar{z}_{61} = z_{61} + z_{78}$ $(T_{ij})_6 = -P_6 \delta_{ij}$
l max	$\frac{M_7}{V_7} = 0, E_{81} = 1$ $\bar{r}_{61} = r_6 - r_1 + r_5 - r_4$ $\bar{z}_{61} = z_6 - z_1 + z_5 - z_4$ $(T_{ij})_7 = -P_7 \delta_{ij}$

2. RIGID WALL

The rigid-wall boundary conditions [Eq. (II-35)] requires continuity of density, zero shear stress, and zero normal component of velocity at the boundary.

If the grid boundary is a rigid wall, then the angle θ that the grid boundary makes with the z axis must be specified. If k zero or k max is a rigid wall (Fig. 4), then θ is the angle between the z axis and the positive l direction at the wall. If l zero or l max is a rigid wall (Fig. 5), then θ is the angle between the z axis and the positive k direction at the wall. In each case, the positive direction for θ is from z toward r .

From Fig. 4 and Eq. (II-44),

$$T_{kk} = T_{rr} \cos^2 \theta + T_{zz} \sin^2 \theta - T_{rz} \sin^2 \theta = -T, \quad (\text{IV-1a})$$

$$T_{kl} = T_{rz} \cos^2 \theta + (T_r - T_z) \sin \theta \cos \theta = F, \quad (\text{IV-1b})$$

$$r_8 - r_1 = R_{81} \sin \theta$$

$$z_8 - z_1 = R_{81} \cos \theta$$

$$R_{81} = \sqrt{(r_8 - r_1)^2 + (z_8 - z_1)^2}, \quad (\text{IV-1c})$$

$$\vec{k} = \cos \theta \vec{e}_r - \sin \theta \vec{e}_z,$$

$$\vec{l} = \sin \theta \vec{e}_r + \cos \theta \vec{e}_z,$$

$$\vec{e}_r = \cos \theta \vec{k} + \sin \theta \vec{l},$$

$$\vec{e}_z = -\sin \theta \vec{k} + \cos \theta \vec{l}, \quad (\text{IV-1d})$$

where $\vec{k}$, $\vec{l}$, $\vec{e}_r$, and $\vec{e}_z$ are unit vectors in the k , l , r , z direction and

$$\vec{e}_r \times \vec{e}_z = \vec{k} \times \vec{l}.$$

Fig. 4. The k rigid wall.

Fig. 5. The l rigid wall.

Substituting (IV-1c) into (III-14) and (III-15) gives

$$\vec{u}_{81} + \vec{v}_{81} = \frac{2R_{81}}{M_7 J_7/V_7 + M_8 J_8/V_8} \left[\frac{\partial}{\partial k} (-T_{rz} \sin \theta + T_{rr} \cos \theta) \vec{e}_r + \frac{\partial}{\partial k} (T_{rz} \cos \theta - T_{zz} \sin \theta)_k \vec{e}_z \right]. \quad (\text{IV-2})$$

Substituting for $\vec{e}_r$ and $\vec{e}_z$ and using (IV-1a) and (IV-1b) gives

$$\vec{u}_{81} + \vec{v}_{81} = \frac{2R_{81}}{M_7 J_7/V_7 + M_8 J_8/V_8} \left[\frac{\partial T_{kl}}{\partial k} \vec{l} + \frac{\partial T_{kk}}{\partial k} \vec{k} \right]. \quad (\text{IV-3})$$

Since the boundary conditions require no motion normal to the boundary, then

$$\frac{\partial T_{kk}}{\partial k} = 0. \quad (\text{IV-4})$$

If $F = T_{kl}$ and since $\vec{l} = \sin \theta \vec{e}_r + \cos \theta \vec{e}_z$, then

$$\begin{aligned} \vec{u}_{81} &= \frac{\vec{r}_{81} (F_7 - F_8)}{M_7 J_7/V_7 + M_8 J_8/V_8} \\ \vec{v}_{81} &= \frac{\vec{z}_{81} (F_7 - F_8)}{M_7 J_7/V_7 + M_8 J_8/V_8}. \end{aligned} \quad (\text{IV-5})$$

If k zero is the rigid wall, then

$$\begin{pmatrix} \bar{r}_{81} = r_8 - r_1 + r_7 - r_6 \\ \bar{z}_{81} = z_8 - z_1 + z_7 - z_6 \end{pmatrix} \quad (IV-6)$$

and the remaining boundary conditions are satisfied, if

$$\begin{aligned} F_7 - F_8 &= 2F_7, \\ \frac{M_7 J_7}{V_7} + \frac{M_8 J_7}{V_8} &= \frac{2M_7 J_7}{V_7}. \end{aligned} \quad (IV-7)$$

Also, if $E_{61} = 0$ then the zones outside the boundary are decoupled from the acceleration calculation in Eqs. (III-16) and (III-17).

Finally, to insure no motion normal to the boundary,

Table 3. Rigid wall boundary conditions.
 $F = (T_{rz} + Q_{rz}) \cos 2\theta$
 $+ (T_r + Q_r - T_z - Q_z) \sin \theta \cos \theta.$

$$\begin{aligned} u_1^{n+1/2} &= u_1^{n-1/2} \\ &+ \Delta t^n \sin \theta [(ud)_1 \sin \theta \\ &+ (vd)_1 \cos \theta] \\ v_1^{n+1/2} &= v_1^{n-1/2} \\ &+ \Delta t^n \cos \theta [(ud)_1 \sin \theta \\ &+ (vd)_1 \cos \theta]. \end{aligned} \quad (IV-8)$$

Boundary	Modification
k zero	$\dot{u}_{81} = \frac{\bar{r}_{81} F_7}{M_7 J_7 / V_7}$ $\dot{v}_{81} = \frac{\bar{z}_{81} F_7}{M_7 J_7 / V_7}$
k max	$\dot{u}_{81} = \frac{-\bar{r}_{81} F_8}{M_8 J_8 / V_8}$ $\dot{v}_{81} = \frac{-\bar{z}_{81} F_8}{M_8 J_8 / V_8}$
l zero	$\dot{u}_{61} = \frac{-\bar{r}_{61} F_7}{M_7 J_7 / V_7}$ $\dot{v}_{61} = \frac{-\bar{z}_{61} F_7}{M_7 J_7 / V_7}$
l max	$\dot{u}_{61} = \frac{\bar{r}_{61} F_6}{M_6 J_6 / V_6}$ $\dot{v}_{61} = \frac{\bar{z}_{61} F_6}{M_6 J_6 / V_6}$

These modifications are consistent with replacing zone 9218 by a zone equal in size and density to 8167, but having a shear stress

$$(T_{kl})_8 = - (T_{kl})_7.$$

The zones 9218 and 2341 are then decoupled from the acceleration calculation if $E_{61} = 0$. Equation (IV-7) insures that only the acceleration component parallel to the wall is saved.

Table 3 gives the required modifications to Eqs. (III-12) through (III-15) for the exterior rigid-wall boundary condition. Equation (IV-7) applies in all cases. The changes for E_{61} , E_{81} , $\bar{r}_{81}$, $\bar{z}_{81}$, $\bar{r}_{61}$, $\bar{z}_{61}$ are the same as in Table 2.

3. SLIP SURFACE

Fig. 6. The plus and minus points on a slip line.

The slip surface boundary conditions Eq. (II-33) require that the normal components of stress and velocity be continuous at the boundary and that the tangential stress component vanish at the boundary. Since the code only allows an internal k line to be a slip surface, we refer to points on the plus side as those points used to complete the zoning on $k+1$ and points on the minus side as those points used to complete the zoning on $k-1$ (Fig. 6). The problem is to move these points in such a way that the boundary conditions are satisfied.

If a coordinate system is attached to a point on the minus side such that $\vec{k}$ is the unit vector normal to the slip line and $\vec{l}$ is the unit vector tangent to the slip line, then

$$\begin{aligned}\vec{l} &= \frac{r_l}{R_l} \vec{e}_r + \frac{z_l}{R_l} \vec{e}_z, & \vec{k} &= \frac{z_l}{R_l} \vec{e}_r - \frac{r_l}{R_l} \vec{e}_z, \\ \sin \theta &= \frac{r_l}{R_l}, & \cos \theta &= \frac{z_l}{R_l},\end{aligned}\quad (\text{IV-9})$$

where

$$r_l = \frac{\partial r}{\partial l}, \quad z_l = \frac{\partial z}{\partial l}, \quad \text{and} \quad R_l = \sqrt{r_l^2 + z_l^2}.$$

Notice that θ is calculated for each point on the slip surface. If $\vec{v}^-$ and $\vec{v}^+$ are velocities of the minus and plus side of the slip line, then

$$\begin{aligned}\vec{v}^- \cdot \vec{k} &= u^- \frac{z_l}{R_l} - v^- \frac{r_l}{R_l} = v_k^-, \\ \vec{v}^+ \cdot \vec{k} &= u^+ \frac{z_l}{R_l} - v^+ \frac{r_l}{R_l} = v_k^+\end{aligned}\quad (\text{IV-10})$$

are the normal components of velocity. Since the normal component of velocity of a point on the slip line must be identical when viewed from the plus or minus side and since the $\vec{k}, \vec{l}$ coordinate system is attached to a minus point (k^-, l^-), we require

$$\frac{d}{dt} (R_l \vec{v}^- \cdot \vec{k}) = \frac{\partial}{\partial t} (R_l \vec{v}^+ \cdot \vec{k}) \Big|_{k^-, l^- \text{ constant}}. \quad (\text{IV-11})$$

Evaluating the left and right sides of Eq. (IV-11) gives

$$\begin{aligned} \frac{d}{dt} (R_\ell \vec{v}^- \cdot \vec{k}) &= a_r^- z_\ell - a_z^- r_\ell + u^- \frac{\partial v^-}{\partial t} - v^- \frac{\partial u^-}{\partial t} \\ &= R_\ell a_k^- + u^- v_\ell^- - v^- u_\ell^- \end{aligned} \quad (IV-12)$$

and

$$\begin{aligned} \frac{\partial}{\partial t} (R_\ell \vec{v}^+ \cdot \vec{k}) &= \frac{d}{dt} (R_\ell \vec{v}^+ \cdot \vec{k}) - \frac{[(u^+ - u^-) \sin \theta + (v^+ - v^-) \cos \theta]}{R_\ell} \frac{(R_\ell \vec{v}^+ \cdot \vec{k})}{\partial \ell} \\ &= R_\ell a_k^+ + u^+ v_\ell^- - v^+ u_\ell^- - [(u^+ - u^-) \sin \theta \\ &\quad + (v^+ - v^-) \cos \theta] [u_\ell^+ \cos \theta - v_\ell^+ \sin \theta] \end{aligned} \quad (IV-13)$$

where subscript ℓ means $\partial/\partial \ell$, subscript k means normal component, terms of the order $\partial \sin \theta / \partial \ell$ have been dropped, and a_k^+ and a_k^- are the normal components of acceleration at the same point on the plus and minus side of the slip line.

Substituting Eqs. (IV-12) and (IV-13) into Eq. (IV-11) gives

$$a_k^+ - a_k^- = [(u^+ - u^-) \sin \theta + (v^+ - v^-) \cos \theta] \left[-\frac{u_\ell^+ + u_\ell^-}{R_\ell} \cos \theta - \frac{v_\ell^+ + v_\ell^-}{R_\ell} \sin \theta \right] = A_c. \quad (IV-14)$$

The term on the left of Eq. (IV-14) is the Coriolis acceleration that results when a particle has a velocity relative to a rotating coordinate system. In order to write Eq. (IV-14) in this form, we have used

$$(u^+ - u^-) \cos \theta - (v^+ - v^-) \sin \theta = 0 \quad (IV-15)$$

which is the continuity of the normal component of velocity boundary condition.

Fig. 7. Interpolated zoning at the slip line.

The plus and minus points are extended to $k-1$ and $k+1$ respectively. These extensions create new zones containing interpolated masses, volumes and stresses. In Fig. 7, if points 4^+ , 1^+ and 8^+ are real points, then zone 921^-8^- and zone 234^-1^- are interpolated zones where the interpolation is performed using the real zones on the minus side. The points 4^- , 1^- and 8^- have interpolated velocities appropriate to the minus side.

Since the plus and minus sides are to be coupled only through the 81 and 14 components of acceleration in Eqs. (III-16) and (III-17), we isolate these components along

with the normal component of stress at the boundary by setting $E_{61} = 0$ on the plus side and $E_{61} = 1$ on the minus side. These modifications are consistent with both the k zero and k max free-surface and rigid-wall boundary conditions. If $E_{61} = 0$ in Eqs. (III-16) and (III-17), then the acceleration of a point on the plus side is given by

$$\begin{aligned}\dot{u}^+ &= E_{81}^+ \dot{u}_{14}^+ + (1 - E_{81}^+) \dot{u}_{81}^+ + E_{81}^+ \dot{u}_6 + (1 - E_{81}^+) \dot{u}_7 + \dot{u}_{61}, \\ \dot{v}^+ &= E_{81}^+ \dot{v}_{14}^+ + (1 - E_{81}^+) \dot{v}_{81}^+ + E_{81}^+ \dot{v}_6 + (1 - E_{81}^+) \dot{v}_7 + \dot{v}_{61}.\end{aligned}\quad (\text{IV-16})$$

The acceleration of a point on the minus side is obtained if $E_{61} = 1$. Therefore,

$$\dot{u}^- = E_{81}^- \dot{u}_{14}^- + (1 - E_{81}^-) \dot{u}_{81}^- + E_{81}^- \dot{u}_1 + (1 - E_{81}^-) \dot{u} + \dot{u}$$

and

$$\dot{v}^- = E_{81}^- \dot{v}_{14}^- + (1 - E_{81}^-) \dot{v}_{81}^- + E_{81}^- \dot{v}_1 + (1 - E_{81}^-) \dot{v}_8 + \dot{v}_{12}.\quad (\text{IV-17})$$

Equations (IV-1), (IV-3), and (IV-6) give

$$(\ddot{u}_{81}^+ + \ddot{v}_{81}^+) \cdot \vec{k} = \frac{2R_{81}^+}{M_7 J_7 / V_7} (-T_7 + P^*),\quad (\text{IV-18a})$$

$$(\ddot{u}_{81}^- + \ddot{v}_{81}^-) \cdot \vec{k} = \frac{2R_{81}^-}{M_8 J_8 / V_8} (-P^* + T_8),\quad (\text{IV-18b})$$

$$(\ddot{u}_{81}^+ + \ddot{v}_{81}^+) \cdot \vec{l} = \frac{2R_{81}^+}{M_7 J_7 / V_7} F_7,\quad (\text{IV-19a})$$

$$(\ddot{u}_{81}^- + \ddot{v}_{81}^-) \cdot \vec{l} = -\frac{2R_{81}^-}{M_8 J_8 / V_8} F_8,\quad (\text{IV-19b})$$

where P^* is the normal component of stress (with compression positive) at the boundary. T and F are defined in Eqs. (IV-1a) and (IV-1b). Equations (IV-18a) and (IV-18b) insure continuity of the normal component of stress at the boundary. Equations (IV-19a) and (IV-19b) make the tangential component of stress zero at the boundary.

If

$$B^+ = \frac{2R_{14}^+}{M_6 J_6 / V_6} E_{81}^+.$$

$$C^+ = \frac{2R_{81}^+}{M_7 J_7 / V_7} (1 + E_{81}^+),$$

$$B^- = \frac{2R_{14}^-}{M_1 J_1 / V_1} E_{81}^-.$$

$$C^- = \frac{2R_{81}^-}{M_8 J_8 / V_8} (1 + E_{81}^-),$$

then

$$a_k^+ = B^+ (P^+ - T_6) + C^+ (P^+ - T_7) + E_{81}^+ \begin{vmatrix} \dot{u}_6 & \dot{v}_6 \\ \sin \theta & \cos \theta \end{vmatrix} + (1 - E_{81}^+) \begin{vmatrix} \dot{u}_7 & \dot{v}_7 \\ \sin \theta & \cos \theta \end{vmatrix} + \begin{vmatrix} \dot{u}_{61} & \dot{v}_{61} \\ \sin \theta & \cos \theta \end{vmatrix}$$

$$a_k^- = B^- (T_1 - P^+) + C^- (T_8 - P^+) + E_{81}^- \begin{vmatrix} \dot{u}_1 & \dot{v}_1 \\ \sin \theta & \cos \theta \end{vmatrix} + (1 - E_{81}^-) \begin{vmatrix} \dot{u}_8 & \dot{v}_8 \\ \sin \theta & \cos \theta \end{vmatrix} + \begin{vmatrix} \dot{u}_{12} & \dot{v}_{12} \\ \sin \theta & \cos \theta \end{vmatrix}$$

where we have assumed that P^+ acts over the entire 48 surface.

Using Eq. (IV-14) to solve for P^+ gives

$$P^+ = \frac{T_6 B^+ + T_7 C^+ + T_1 B^- + T_8 C^- + A}{B^+ + C^+ + B^- + C^-} \quad (IV-20)$$

where

$$A = A_c + E_{81}^- \begin{vmatrix} \dot{u}_1 & \dot{v}_1 \\ \sin \theta & \cos \theta \end{vmatrix} - E_{81}^+ \begin{vmatrix} \dot{u}_6 & \dot{v}_6 \\ \sin \theta & \cos \theta \end{vmatrix} + (1 - E_{81}^-) \begin{vmatrix} \dot{u}_8 & \dot{v}_8 \\ \sin \theta & \cos \theta \end{vmatrix} - (1 - E_{81}^+) \begin{vmatrix} \dot{u}_7 & \dot{v}_7 \\ \sin \theta & \cos \theta \end{vmatrix} + \begin{vmatrix} \dot{u}_{12} - \dot{u}_{61} & \dot{v}_{12} - \dot{v}_{61} \\ \sin \theta & \cos \theta \end{vmatrix}$$

If a point on the plus side is to be moved, i.e., 1^+ is a real point in Fig. 7, then

$$(a_k^+)_{14+81} = P^+ (C^+ + B^+) - T_6 B^+ - T_7 C^+,$$

$$\dot{u}_k^+ = [(a_k^+)_{14+81}] \cos \theta,$$

$$\dot{v}_k^+ = -[(a_k^+)_{14+81}] \sin \theta,$$

$$\dot{u}_{81}^+ = \frac{2R_{81}^+ F_7}{M_7 J_7 / V_7} \sin \theta,$$

$$\dot{v}_{81}^+ = \frac{2R_{81}^+ F_7}{M_7 J_7 / V_7} \cos \theta,$$

and

$$\begin{aligned} (ud)_1^+ &= \dot{u}_k^+ + E_{81}^+ \dot{u}_{14}^+ + (1 - E_{81}^+) \dot{u}_{81}^+ + E_{81}^- \dot{u}_6 + (1 - E_{81}^+) \dot{u}_7 + \dot{u}_{61} + f_r + QKL_r, \\ (vd)_1^+ &= \dot{u}_k^+ + E_{81}^+ \dot{v}_{14}^+ + (1 - E_{81}^+) \dot{v}_{81}^+ + E_{81}^+ \dot{v}_6 + (1 - E_{81}^+) \dot{v}_7 + \dot{v}_{61} + f_z + QKL_z. \end{aligned} \quad (IV-21)$$

If a point on the minus side is to be moved, i.e., 1^- is a real point in Fig. 7, then

$$\begin{aligned} (a_k^-)_{14+81} &= B^- T_1 + C^- T_8 - P^* (B^- + C^-), \\ \dot{u}_k^- &= [(a_k^-)_{14+81}] \cos \theta, & \dot{v}_k^- &= -[(a_k^-)_{14+81}] \sin \theta, \\ \dot{u}_{61}^- &= \frac{-2R_{81}^- F_8}{M_8 J_8 / V_8} \sin \theta, & \dot{v}_{81}^- &= -\frac{2R_{81}^- F_8}{M_8 J_8 / V_8} \cos \theta, \end{aligned}$$

and

$$\begin{aligned} (ud)_1^- &= \dot{u}_k^- + E_{81}^- \dot{u}_{14}^- + (1 - E_{81}^-) \dot{u}_{81}^- + E_{81}^- \dot{u}_1 + (1 - E_{81}^-) \dot{u}_8 + \dot{u}_{12} + f_r + QKL_r, \\ (vd)_1^- &= \dot{v}_k^- + E_{81}^- \dot{v}_{14}^- + (1 - E_{81}^-) \dot{v}_{81}^- + E_{81}^- \dot{v}_1 + (1 - E_{81}^-) \dot{v}_8 + \dot{v}_{12} + f_z + QKL_z. \end{aligned} \quad (IV-22)$$

After all the points on both the plus and minus side of the slip line have been moved using Eqs. (IV-21) and (IV-22) those points on the slave side are moved normal to the master side until they fall on the master side. The normal component of velocity of the points on the slave side is then recalculated as an interpolated master side velocity. The master side (either plus or minus) is specified in the generator and usually corresponds to the material side that is expected to move the least.

V. The Strain Calculations

The strain rate tensor given by Eqs. (II-76) and (II-80) of section II may be written

$$\begin{pmatrix} e_{rr} & 0 & e_{rz} \\ 0 & e_{\phi\phi} & 0 \\ e_{rz} & 0 & e_{zz} \end{pmatrix} = \frac{1}{3} \begin{pmatrix} e & 0 & 0 \\ 0 & e & 0 \\ 0 & 0 & e \end{pmatrix} + \begin{pmatrix} e_r & 0 & e_{rz} \\ 0 & e_\phi & 0 \\ e_{rz} & 0 & e_z \end{pmatrix} \quad (V-1)$$

where

$$\Theta = e_{rr} + e_{\phi\phi} + e_{zz} = V^{-1} \frac{dV}{dt}, \quad (V-2a)$$

$$e_r = e_{rr} - \frac{\Theta}{3} = \frac{1}{3} \left(2 \frac{\partial u}{\partial r} - \frac{\partial v}{\partial z} - \frac{u}{r} \right), \quad (V-2b)$$

$$e_\phi = e_{\phi\phi} - \frac{\Theta}{3} = - (e_r + e_z), \quad (V-2c)$$

$$e_z = e_{zz} - \frac{\Theta}{3} = - \frac{1}{3} \left(2 \frac{\partial v}{\partial z} - \frac{\partial u}{\partial r} - \frac{u}{r} \right), \quad (V-2d)$$

$$e_{rz} = \frac{1}{2} \left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r} \right). \quad (V-2e)$$

In the code the above strain rates are calculated using time-centered zone coordinates at $t^{n+1/2}$ and coordinate velocities $u^{n+1/2}$ and $v^{n+1/2}$. Using $(ud)_1^n$ and $(vd)_1^n$ from section IV, zone velocities and coordinates are calculated as follows:

$$u_1^{n+1/2} = u_1^{n-1/2} + \Delta t^n (ud)_1^n$$

$$v_1^{n+1/2} = v_1^{n-1/2} + \Delta t^n (vd)_1^n$$

$$r_1^{n+1} = r_1^n + \Delta t^{n+1/2} u_1^{n+1/2}$$

$$z_1^{n+1} = z_1^n + \Delta t^{n+1/2} v_1^{n+1/2}$$

$$\Delta r_1^{n+1} = \Delta r_1^n + u_1^{n+1/2} \Delta t^{n+1/2}$$

$$\Delta z_1^{n+1} = \Delta z_1^n + v_1^{n+1/2} \Delta t^{n+1/2}$$

$$r_1^{n+1/2} = r_1^n + \frac{u_1^{n+1/2} \Delta t^{n+1/2}}{2} = r_1^{n+1} - \frac{u_1^{n+1/2} \Delta t^{n+1/2}}{2}$$

$$z_1^{n+1/2} = z_1^n + \frac{v_1^{n+1/2} \Delta t^{n+1/2}}{2} = z_1^{n+1} - \frac{v_1^{n+1/2} \Delta t^{n+1/2}}{2}$$

In the remainder of this section, if the superscript is omitted it is understood to be $n+1/2$. Also, we define

$$r_{76} = r_7 - r_6, \quad z_{76} = z_7 - z_6, \quad r_{781} = r_7 + r_8 + r_1, \text{ etc.}$$

If we consider a typical zone, say 8167 in Fig. 3a, the zone volume is calculated explicitly at cycle zero (the beginning of the problem) as

$$V_7^0 = r_{781}^0 \begin{vmatrix} r_{78}^0 & r_{71}^0 \\ z_{78}^0 & z_{71}^0 \end{vmatrix} + r_{761}^0 \begin{vmatrix} r_{71}^0 & r_{76}^0 \\ z_{71}^0 & z_{76}^0 \end{vmatrix} = \frac{3}{\pi} \times (\text{zone volume})$$

if

$$\Delta V_7 = V_7^{n+1} - V_7^n. \quad (V-3)$$

Then, substituting

$$\begin{aligned} r^{n+1} &= r + \frac{\Delta t}{2} u, & z^{n+1} &= z + \frac{\Delta t}{2} v, \\ r^n &= r - \frac{\Delta t}{2} u, & z^n &= z - \frac{\Delta t}{2} v, \end{aligned}$$

into Eq. (V-3) gives

$$\begin{aligned} \Delta V_7^{n+1/2} &= \Delta t \left\{ u_{781} \begin{vmatrix} r_{78} & r_{71} \\ z_{78} & z_{71} \end{vmatrix} + u_{716} \begin{vmatrix} r_{71} & r_{76} \\ z_{71} & z_{76} \end{vmatrix} + r_{781} \begin{vmatrix} u_{78} & u_{71} \\ z_{78} & z_{71} \end{vmatrix} + r_{716} \begin{vmatrix} u_{71} & u_{76} \\ z_{71} & z_{76} \end{vmatrix} \right. \\ &\quad + r_{781} \begin{vmatrix} r_{78} & r_{71} \\ v_{78} & v_{71} \end{vmatrix} + r_{716} \begin{vmatrix} r_{71} & r_{76} \\ v_{71} & v_{76} \end{vmatrix} \\ &\quad \left. + \left(\frac{\Delta t}{2} \right)^2 \left[u_{781} \begin{vmatrix} u_{78} & u_{71} \\ v_{78} & v_{71} \end{vmatrix} + u_{761} \begin{vmatrix} u_{71} & u_{76} \\ v_{71} & v_{76} \end{vmatrix} \right] \right\}. \quad (V-4) \end{aligned}$$

Then,

$$\begin{aligned} DV_7^{n+1} &= DV_7^n + \Delta V_7^{n+1/2} \\ V_7^{n+1} &= V_7^0 + DV_7^{n+1} \\ V_7^{n+1/2} &= V_7^{n+1} - \frac{\Delta V_7^{n+1/2}}{2}. \quad (V-5) \end{aligned}$$

$$MU_7^{n+1} = - \frac{DV_7^{n+1}}{V_7^{n+1}} \quad (V-6)$$

$$\eta_7^{n+1} = \frac{V_7^0}{V_7^{n+1}} \quad (V-7)$$

$$EDV_7 = \frac{\Delta V_7^{n+1/2}}{V_7^0} \quad (V-8)$$

Equation (V-6) is defined to be the total volumetric strain associated with zone 8167. Notice that the code has not used Eq. (V-2a) to calculate volume changes. Equation (V-4) is exact in that it represents no assumption concerning the differenced form of the partial derivatives.

The relation between Θ and MU is given by

$$\int \Theta dt = \ln v/v_0.$$

$$e^{-\int \Theta dt} = MU + 1.$$

If the exponent is small so that higher order terms can be neglected in the $e^{-\int \Theta dt}$ expansion, then

$$\int \Theta dt = -MU. \quad (V-9)$$

The zone area J at t^{n+1} and $t^{n+1/2}$ is calculated as

$$2J^{n+1} = \begin{vmatrix} r_{71}^{n+1} & r_{86}^{n+1} \\ z_{71}^{n+1} & z_{86}^{n+1} \end{vmatrix} \quad 2J^{n+1/2} = \begin{vmatrix} r_{71} & r_{86} \\ z_{71} & z_{86} \end{vmatrix} \quad (V-10)$$

The deviatoric strain rates [e_r , e_z , e_{rz} in Eq. (V-2)] can be transformed into the Lagrangian coordinate system using Eqs. (III-3) and (III-4),

$$\begin{aligned} \frac{\partial u}{\partial r} &= \frac{1}{4J^{n+1/2}} \left[(u_{71} - u_{86})(z_{71} + z_{86}) - (u_{71} + u_{86})(z_{71} - z_{86}) \right] \\ &= \frac{1}{2J^{n+1/2}} \begin{vmatrix} u_{71} & u_{86} \\ z_{71} & z_{86} \end{vmatrix}, \end{aligned} \quad (V-11a)$$

$$\frac{\partial u}{\partial z} = \frac{1}{2J^{n+1/2}} \begin{vmatrix} u_{86} & u_{71} \\ r_{86} & r_{71} \end{vmatrix}, \quad (V-11b)$$

$$\frac{\partial v}{\partial r} = \frac{1}{2J^{n+1/2}} \begin{vmatrix} v_{71} & v_{86} \\ z_{71} & z_{86} \end{vmatrix}, \quad (V-11c)$$

$$\frac{\partial v}{\partial z} = \frac{1}{2J^{n+1/2}} \begin{vmatrix} v_{86} & v_{71} \\ r_{86} & r_{71} \end{vmatrix}, \quad (V-11d)$$

$$\frac{u}{r} = \frac{u_8 + u_1 + u_6 + u_7}{r_8 + r_1 + r_6 + r_7}. \quad (V-11e)$$

When Eqs. (V-11a) through (V-11e) are substituted into (V-2b), (V-2d), and (V-2e), the deviatoric strain rates for zone 8167 become available at time $t^{n+1/2}$. The change in deviatoric strain between t^n and t^{n+1} is

$$\Delta e_r = e_r \Delta t^{n+1/2}, \quad (V-12)$$

$$\Delta e_z = e_z \Delta t^{n+1/2}, \quad (V-13)$$

$$\Delta e_{rz} = e_{rz} \Delta t^{n+1/2}. \quad (V-14)$$

The rigid-body rotation of the zone during the same time increment is given by¹⁹

$$\Delta \Phi = \frac{\Delta t^{n+1/2}}{2} \left(\frac{\partial u}{\partial z} - \frac{\partial v}{\partial r} \right). \quad (V-15)$$

where the positive direction for Φ is from z toward r .

The basic strain increments used in the code are given by Eqs. (V-4) and (V-12) through (V-15). The only total strain component calculated by the code is that associated with the volumetric strain [Eq. (V-6)]. Total deviatoric strains are not saved. The rigid-body rotation of a zone [Eq. (V-15)] is not a strain. However, since the stress tensor is assumed to experience the same rotation as the zone, $\Delta \Phi$ will be used to decouple the stress tensor from the rigid-body rotation.

The minimum dimension ΔL of a zone will be required in the next two sections. From Eq. (III-6) and Fig. 3b we find that if

$$|\vec{R}_k| > |\vec{R}_\ell|$$

then

$$\Delta L = |\vec{R}_\ell| \sin \theta = \frac{J}{|\vec{R}_k|}.$$

However, if

$$|\vec{R}_f| > |\vec{R}_k|$$

then

$$\Delta L = |\vec{R}_k| \sin \theta = \frac{J}{|\vec{R}_f|}.$$

For zone 8167, we have

$$|\vec{R}_k|^2 = \left(\frac{r_{61} + r_{78}}{2} \right)^2 + \left(\frac{z_{61} + z_{78}}{2} \right)^2,$$

$$|\vec{R}_f|^2 = \left(\frac{r_{76} + r_{81}}{2} \right)^2 + \left(\frac{z_{76} + z_{81}}{2} \right)^2,$$

$$R^2 = \text{Maximum} (|\vec{R}_k|^2, |\vec{R}_f|^2),$$

$$\Delta L_7 = \frac{J_7}{R}.$$

(V-16)

VI. The Equation of State

The equation of state (EOS) allows the strain increments calculated in section V to be converted into stresses. The EOS section of the code has been designed to accept, in table form, the results of laboratory tests on rock samples.

The experimental procedures required to obtain the test data are given by Stephens,⁵ Schock,⁶ Heard⁷ and Murri and Smith.²⁰ The reduction of the test data into an EOS formulation has been given by Cherry and Petersen.²¹ We assume that the reader is familiar at least with Ref. 21 so the justification of the EOS formulation and its development for a particular site will not be given here.

1. STRAIN RATE, STRESS RATE AND HOOKE'S LAW

The form of the strain rate tensor e_{ij} , defined by Eq. (II-75), is obtained from the conservation of energy formulation and the symmetry of the stress tensor. It is easy to show that e_{ij} measures the rate of separation experienced by two adjacent particles.

If we consider two particles whose coordinates and velocities in a Cartesian coordinate system^{*} are y^i , $y^i + dy^i$, u_i , $u_i + du_i$ and if ds is the scalar distance between the particles, then

$$\lim_{\Delta t \rightarrow 0} \frac{[(ds)_{t+\Delta t}^2 - (ds)_t^2]}{\Delta t} = 2du_i dy^i. \quad (VI-1)$$

Since at any given time

$$du_i = \frac{\partial u_i}{\partial y^j} dy^j, \quad (VI-2)$$

then

$$\frac{d(ds)^2}{dt} = 2 \frac{\partial u^i}{\partial y^j} dy^j dy^i. \quad (VI-3)$$

If we define

$$e_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial y^j} + \frac{\partial u_j}{\partial y^i} \right) \quad (VI-4)$$

and

$$\omega_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial y^j} - \frac{\partial u_j}{\partial y^i} \right), \quad (VI-5)$$

then

$$\frac{\partial u^i}{\partial y^j} = e_{ij} + \omega_{ij} \quad (VI-6)$$

and

$$\omega_{ij} dy^j dy^i = 0 \quad (\text{since } \omega_{ij} \text{ is antisymmetric}). \quad (VI-7)$$

Substituting Eqs. (VI-6) and (VI-7) into (VI-3) gives

$$\frac{d(ds)^2}{dt} = 2e_{ij} dy^j dy^i. \quad (VI-8)$$

If the line element joining the two particles rotates so that $(ds)^2$ is constant, then by Eq. (VI-8) e_{ij} must vanish. This means that e_{ij} is insensitive to the instantaneous rotation of the line element. Also, since Eq. (VI-7) must be satisfied for any type of deformation, ω_{ij} is the rotation rate tensor. Therefore,

*The results obtained for Cartesian coordinates may easily be extended to curvilinear fixed-point coordinates by using the tensor notation of section II.9.

$$du_i = e_{ij} dy^j + \omega_{ij} dy^j = du_i^{**} + du_i^*$$

where

$$du_i^* = \omega_{ij} dy^j \quad (VI-9)$$

gives the relative component of velocity normal to the line element joining the two particles, and

$$du_i^{**} = e_{ij} dy^j \quad (VI-10)$$

gives the relative component of velocity parallel to the line element joining the two particles.

The equation of state requires a functional relation between the strain rate and "stress rate". Since the strain rate vanishes during a rigid-body rotation, the "stress rate" definition must allow the Eulerian components of the stress tensor to change during this rotation, even though no strain is occurring.

It is easy to see that the material derivative [Eq. (II-55)] will not be a good "stress rate" definition. If we use a Cartesian coordinate system and write

$$T_{ij} = T_{ij}^0 + \epsilon_{ij}$$

then T_{ij} will be constant when ϵ_{ij} equals zero. Obviously, T_{ij} cannot be constant during a rigid-body rotation (the body rotates, not the coordinate system). Therefore, the material derivative is not a good stress-rate definition.

Apparently, there are almost as many "stress rate" definitions as there are continuum mechanics - thermodynamics authors. If you have enough courage, try Ref. 22, pp. 334-343. The simplest and the one we use is the Jaumann derivative. This derivation is illustrated by Prager²¹ for Cartesian tensors.

Since we wish to exclude the effect of the rotation tensor ω_{ij} on the stress tensor, we consider two coordinate systems γ^i and Y^i having a typical particle as their common origin. The coordinate system γ^i is fixed in space, while the coordinate system Y^i participates only in the rotation of the neighborhood of the particle. If the two coordinate systems are coincident at time t and if T^{ij} and τ^{ij} are the stress tensors in the fixed and rotating coordinates, then at time t

$$\tau_{ij}^{(t)} = T_{ij}^{(t)}$$

and

$$dY^i_{(t)} = dy^i_{(t)} + dY^i_{(t-dt)}$$

At time $t + dt$, we use Eq. (VI-9) to find the new coordinates of the neighboring "particle" to be

$$dy_{(t+dt)}^i = dy_{(t)}^i + \omega_{\cdot j}^i dt dy_{(t)}^j = (\delta_j^i - \omega_{\cdot j}^i dt) dy_{(t+dt)}^j.$$

Therefore, using Eq. (II-42b)

$$\gamma_j^i = (\delta_j^i - \omega_{\cdot j}^i dt)$$

and we find

$$\begin{aligned} \tau_{ij}^{(t+dt)} &= \left(\delta_i^m - \omega_{i\cdot}^m dt \right) \left(\delta_j^n - \omega_{j\cdot}^n dt \right) \left[T_{mn}^{(t)} + \left(-\frac{\delta T_{mn}}{\delta t} \right) dt \right] \\ &= T_{ij}^{(t)} + \left(-\frac{\delta T_{ij}}{\delta t} - \omega_{i\cdot}^m T_{mj} - \omega_{j\cdot}^m T_{im} \right) dt + O(dt^2). \end{aligned}$$

The stress rate in the rotating coordinate system can now be written in terms of the components of stress in the fixed coordinate system as

$$\frac{\tau_{ij}^{(t+dt)} - \tau_{ij}^{(t)}}{dt} \equiv \dot{T}_{ij} = \frac{\delta T_{ij}}{\delta t} - \omega_{i\cdot}^m T_{mj} - \omega_{j\cdot}^m T_{im}. \quad (VI-11)$$

We use Eq. (VI-11) as the stress rate definition where

$$\omega_{ij} = \frac{1}{2} (u_{i,j} - u_{j,i}). \quad (VI-12)$$

Now if the stress rate—strain rate relation is written

$$\dot{T}_{ij} = F(e_{ij}),$$

then T_{ij} will change properly during a rigid-body rotation.

We may now write Hooke's Law for an isotropic material in a stress rate—strain rate form as

$$\frac{\delta T_{ij}^i}{\delta t} = \lambda \theta \delta_j^i + 2\mu e_{ij}^i + T_{\cdot m}^i \omega_{j\cdot}^m + T_{\cdot j}^m \omega_{i\cdot}^m \quad (VI-13)$$

where λ and μ are the Lamé constants (μ is called the shear modulus) and

$$\theta = e_{m}^m = V^{-1} \frac{dV}{dt}. \quad [\text{Eq. (II-80)}] \quad (VI-14)$$

We can use Eq. (VI-13) to find

$$\frac{\delta (T_{m}^m)}{\delta t} = \frac{d(T_{m}^m)}{dt} = (3\lambda + 2\mu) \theta. \quad (VI-15)$$

If the coordinate system is orthogonal, then Eqs. (II-52) and (II-55) apply. Equations (VI-14) and (VI-15) can be written using physical components of the stress tensor and strain-rate tensor as

$$\theta = e_{\alpha\alpha} + e_{\beta\beta} = e_{jj},$$

$$T_{.1}^1 + T_{.2}^2 + T_{.3}^3 = T_{\alpha\alpha} + T_{\beta\beta} + T_{rr} = -3P, \quad (VI-16)$$

$$\frac{dP}{dt} = -\kappa \theta \quad (VI-17)$$

where

$$\kappa \equiv \lambda + \frac{2}{3}\mu \quad (\kappa \text{ is called the bulk modulus}).$$

Equation (VI-17) shows that the rate of mean stress change is proportional to the product of the bulk modulus and the dilatation rate. The rotation correction does not influence this stress component.

In cylindrical coordinates with $u_\phi = 0$ and axial symmetry, we have found $u_\phi = T_{\phi r} = T_{\phi z} = e_{\phi z} = e_{r\phi} = 0$. Also, from Eq. (VI-12), $\omega_{12} = \omega_{23} = 0$. Applying these conditions to Eq. (VI-13) and reducing the tensors to physical components, we find

$$\frac{dT_{rr}}{dt} = \lambda \theta + 2\mu e_{rr} + 2T_{rz} \omega_{rz}, \quad (VI-18a)$$

$$\frac{dT_{\phi\phi}}{dt} = \lambda \theta + 2\mu e_{\phi\phi}, \quad (VI-18b)$$

$$\frac{dT_{zz}}{dt} = \lambda \theta + 2\mu e_{zz} - 2T_{rz} \omega_{rz}, \quad (VI-18c)$$

$$\frac{dT_{rz}}{dt} = 2\mu e_{rz} + (T_{zz} - T_{rr}) \omega_{rz}, \quad (VI-18d)$$

where the physical component ω_{rz} of the rotation rate tensor is

$$\omega_{rz} = \frac{1}{2} \left(\frac{\partial u_r}{\partial z} - \frac{\partial u_z}{\partial r} \right). \quad (VI-19)$$

Notice in Eq. (VI-18) that the material derivative of the components of the stress tensor has reduced to the Lagrangian derivative. The Christoffel symbols give no contribution due to the imposed axial symmetry and the vanishing of the u_ϕ component of velocity.

Finally, if Eqs. (VI-17) and (VI-18) are combined, then Hooke's Law can be written in terms of mean stress and deviatoric stress components as

$$\frac{dP}{dt} = -\kappa \Theta, \quad (VI-20)$$

$$\frac{dT_r}{dt} = 2\mu e_r + 2T_{rz} \omega_{rz}, \quad (VI-21)$$

$$\frac{dT_z}{dt} = 2\mu e_z - 2T_{rz} \omega_{rz}, \quad (VI-22)$$

$$\frac{dT_{rz}}{dt} = 2\mu e_{rz} + (T_z - T_r) \omega_{rz}, \quad (VI-23)$$

where

$$\begin{aligned} T_r &= T_{rr} + P, & \Theta &= e_{rr} + e_{\phi\phi} + e_{zz}, \\ T_z &= T_{zz} + P, & e_r &= e_{rr} - \frac{\Theta}{3}, \\ T_\phi &= T_{\phi\phi} + P = -(T_r + T_z), & e_z &= e_{zz} - \frac{\Theta}{3}, \\ & & e_\phi &= e_{\phi\phi} - \frac{\Theta}{3} = -(e_r + e_z). \end{aligned} \quad (VI-24)$$

The deviatoric strain rates, e_r , e_z , and e_{rz} , have been written in Eq. (V-2) for our symmetry conditions. The differenced form of the terms required to obtain a given deviatoric strain rate are given in Eqs. (V-11a) through (V-11e). Using Eqs. (V-12) through (V-15), the stress deviators at time t^{n+1} can be found by

$$\bar{T}_r^{n+1} = T_r^n + 2\mu \Delta e_r + 2T_{rz}^n \Delta\phi, \quad (VI-25a)$$

$$\bar{T}_z^{n+1} = T_z^n + 2\mu \Delta e_z - 2T_{rz}^n \Delta\phi, \quad (VI-25b)$$

$$\bar{T}_{rz}^{n+1} = T_{rz}^n + 2\mu \Delta e_{rz} + (T_z^n - T_r^n) \Delta\phi. \quad (VI-25c)$$

The terms that correct for the zone rotation are a half-cycle off; i.e., the stresses multiplying $\Delta\phi$ in the above equations should correspond to time $n+1/2$ instead of n .

Equation (VI-25) represents the initial attempt by the code to calculate the stress deviators. Adjustment of these stress components is permitted if the zone is undergoing plastic flow or brittle failure.

2. THE CALCULATION OF MEAN STRESS

In the code, Eq. (VI-20) is replaced by

$$P = f(\text{MU}, e) \quad (VI-26)$$

where

MU is the total volumetric strain [Eq. (V-6)] and

e is the total internal energy/original volume. The relationship between ϵ of section II.3 and e is

$$e = \rho^0 \epsilon.$$

The form of Eq. (VI-26) depends on the state of the material. During shock loading, Eq. (VI-26) becomes

$$P_H^{n+1} = f_H (MU^{n+1}), \quad (VI-27)$$

where f_H is determined from hydrostatic compressibility and Hugoniot measurements on core samples.

Equations (II-36), (II-37a), and (II-39) give the Hugoniot jump conditions. The normal component of stress T_{11} in these equations is composed of mean stress (P) and deviatoric (T_1) components ($T_{11} = -P + T_1$). To obtain Eq. (VI-27) in a form consistent with the EOS model, the laboratory Hugoniot data must be modified so that P versus μ is obtained instead of T_{11} versus MU. The difference between the Hugoniot data and the hydrostatic compressibility data at a common MU may be used to reduce the Hugoniot measurements to mean stress. This difference should be consistent with the material strength inferred from triaxial compression measurements.

The mean stress calculation during release depends on the maximum compression seen by the zone during shock loading. If $MU^{\max}$ is the maximum zone compression, then Eq. (II-39) may be used to calculate the internal energy ($e^{\max}$) associated with this shock state.

If $e_f^I < e^{\max}$, the pressure on release is calculated by

$$P_H^{n+1} = P_H^{n+1} + \Gamma (e^n - e_H)$$

where

P_H^{n+1} is the Hugoniot pressure that corresponds to MU^{n+1} ,

e^n is the internal energy at t^n (e^n should be replaced by e^{n+1} ; however, since this is only used on release, the approximation is not too bad.)

$$e_H = \frac{1}{2} P_H^{n+1} \frac{MU^{n+1}}{1 + MU^{n+1}},$$

$$\Gamma = \Gamma^I \left[\frac{e^{\max} - e_f^I}{e_v^I - e_f^I} \right].$$

The quantities Γ^I , e_p^I , e_v^I are specified in the equation of state.

If the hydrostatic compressibility data indicate that the material locks in the P-MU plane on release, the code will accept one input release path in the equation of state. This release path is usually an experimentally determined hydrostatic unloading path.

The point in the P-MU plane where the experimental loading and unloading hydrostats merge, MU_2^I , is input in the equation of state. If $MU^{\max} \geq MU_2^I$, the release path follows the input unloading curve. If $MU^{\max} < MU_2^I$, the release path is determined such that

$$\left(\frac{dP}{dMU}\right)^{n+1/2} = \left(\frac{dP}{dMU}\right)_L + \frac{MU^{\max}}{MU_2^I} \left[\left(\frac{dP}{dMU}\right)_u - \left(\frac{dP}{dMU}\right)_L \right]$$

where $\left(\frac{dP}{dMU}\right)_L$ and $\left(\frac{dP}{dMU}\right)_u$ are the slopes of the loading and unloading hydrostats for a given P^n . The pressure on release becomes

$$P^{n+1} = P^n - \left(\frac{dP}{dMU}\right)^{n+1/2} \frac{V^0 \Delta V^{n+1/2}}{V^{n+1} (V^{n+1} - \Delta V^{n+1/2})}.$$

3. FAILURE

Three invariants are associated with a second-order symmetric tensor. The material derivative of these invariants reduces to the Lagrangian derivative. We have used this in Eq. (VI-15) for the first invariant of the stress tensor.

For the stress tensor, the invariants are

$$I_1 = T_m^m = -3P \quad I_2 = \frac{1}{2} (I_1^2 - T_n^m T_m^n) \quad I_3 = \left| T_n^m \right|.$$

In Ref. 21 a failure criterion was presented, in terms of stress invariants, that attempted to describe the onset of failure in brittle materials. The invariants used were the mean stress (P), the second deviatoric invariant (I_{2D}), and the third deviatoric invariant (I_{3D}). In terms of the physical components of our stress tensor,

$$I_{2D} = T_r^2 + T_z^2 + T_r T_z + T_{rz}^2,$$

$$I_{3D} = (T_r + T_z) (T_{rz}^2 - T_r T_z).$$

If the material strength Y is represented by

$$Y = \left(\frac{3}{4} I_{2D} \right)^{1/2}$$

and the stress state $\bar{P}$ by

$$\bar{P} = P - \frac{1}{2} \left(\frac{I_{3D}}{2} \right)^{1/3},$$

then a consistent failure surface resulted in Ref. 21 when the results of various destructive tests (tension, triaxial compression and triaxial extension) were plotted as Y versus $\bar{P}$.

The onset of zone failure in the code is determined by a table of Y versus $\bar{P}$. The table is usually obtained from triaxial compression test data, the tensile strength and the Hugoniot elastic limit, where Y and $\bar{P}$ are evaluated for each test.

Adjustment of the deviatoric stresses calculated in Eq. (VI-25) is permitted if the zone is undergoing plastic flow or brittle failure. The code uses two strength tables, one for the consolidated and one for the cracked state, a strain rate value Y^I and a brittle-ductile transition point $\bar{P}^I$.

If $\bar{P}^{n+1} \geq \bar{P}^I$ and if $Y^{n+1} > (E)(Y^I)$, then plastic flow develops. The deviatoric stress adjustment is

$$T_{\alpha}^{n+1} = \left(\frac{(E)(Y^I)}{Y^{n+1}} \right) T_{\alpha}^{n+1}, \quad \text{where } \alpha \text{ is } r, z, rz \quad (\text{VI-28})$$

and

$$E = \frac{e_f^I - e^n}{e_f^I} = 0, \quad \text{if } e_f^I < e^n.$$

If $\bar{P} < \bar{P}^I$ and if Y^{n+1} is greater than the value of Y allowed by the appropriate strength table, a crack is allowed to propagate through a zone with a velocity C_v , given by

$$C_v = 1.14 \sqrt{\frac{\mu}{\rho \left(3 + \frac{\mu}{k} \right)}}.$$

A crack length C_L and a crack ratio C_R are calculated as

$$C_L^{n+1} = C_L^n + C_v \Delta t^{n+1/2}$$

and

$$C_R = \frac{C_L^{n+1}}{4 \Delta L^{n+1}} \leq 1 \quad (\text{the crack stops when } C_R = 1).$$

A limiting value of Y is calculated as

$$Y_{\text{Lim}} = Y^{n+1} \left[1 - \frac{C_v C_R \Delta t^{n+1/2}}{4 \Delta L} \right] \leq Y^I \quad [\Delta L \text{ is given by Eq. (V-16).}] \quad (\text{VI-29})$$

Equation (VI-28) is used to calculate the adjusted deviatoric stress components, with Y^I replaced by Y_{Lim} .

During plastic flow, the stress adjustment is made normal to the yield surface with the yield surface defined by

$$Y = (E)(Y^I).$$

During brittle failure, the adjustment is modeled after a Maxwell solid with the viscosity η given by

$$\eta = \frac{4\mu\Delta L}{C_v C_R}.$$

In both cases, the adjusted deviatoric stress components are obtained by simple scaling.

At the present time we are using the code to simulate the triaxial compression test on granite. The modifications in the failure routine required to match the results of the numerical model with observed stress-strain measurements will be the subject of a later paper.

VII. Energy, Damping and Δt Calculations

1. INTERNAL ENERGY AND KINETIC ENERGY

The differential form of the conservation of energy has been written in Eq. (II-78), as

$$\rho \frac{d\epsilon}{dt} = T_{rr} e_{rr} + T_{zz} e_{zz} + T_{\phi\phi} e_{\phi\phi} + 2T_{rz} e_{rz}. \quad (\text{VII-1})$$

Since

$$T_{rr} = -P + T_r, \text{ etc.},$$

$$e_{rr} = V^{-1} \frac{dV}{dt} + e_r, \text{ etc.},$$

$$T_r + T_\phi + T_z = e_r + e_\phi + e_z = 0.$$

Then Eq. (VII-1) can be written

$$\frac{V^0}{V} \frac{de}{dt} = -\frac{P}{V} \frac{dV}{dt} + (2T_r + T_z)e_r + (2T_z + T_r)e_z + 2T_{rz}e_{rz} \quad (\text{VII-2})$$

where

$$e = \rho^0 \epsilon.$$

In differenced form, Eq. (VII-2) becomes

$$e_7^{n+1} = e_7^n - \bar{P}(\text{EDV}) + \frac{V^{n+1/2}}{V^c} \left[(2T_r + T_z)\Delta e_r + (2T_z + T_r)\Delta e_z + 2T_{rz}\Delta e_{rz} \right] \quad (\text{VII-3})$$

where EDV is given by Eq. (V-8) and the strain increments by Eqs. (V-12), (V-13), and (V-14). In Eq. (VII-3),

$$\bar{P} = \frac{P^{n+1} + P^n}{2} + Q^{n+1/2} \quad \bar{T}_r = \frac{T_r^{n+1} + T_r^n}{2} + Q_r^{n+1/2}, \text{ etc.}$$

The kinetic energy of a zone is calculated as

$$K_7^{n+1/2} = \frac{M_7}{32} [(u_8 + u_1 + u_6 + u_7)^2 + (v_8 + v_1 + v_6 + v_7)^2]. \quad (\text{VII-4})$$

Equation (II-12) becomes

$$K + E = \frac{\pi}{3} \sum_{k,\ell} (v_7^0 e_7^{n+1} + K_7^{n+1/2}). \quad (\text{VII-5})$$

In the energy sum of Eq. (VII-5), the internal and kinetic energies are 1/2 cycle off.

2. DAMPING

A typical zone may develop a maximum of six Q terms. A Q term is associated with each stress component. These are Q_x, Q_y, Q_z, Q_{xz} where Q is added to P , Q_x is added to T_x , Q_y is added to T_y and Q_{xz} is added to T_{xz} . In addition, there are two Q components that are designed to oppose translation of zone diagonals. These are called QKL_x and QKL_y .

The Q associated with the mean stress is calculated as follows: For a given zone, say 8167, we define

$$F_k = \frac{\partial F}{\partial k} = \frac{1}{2} (F_7 + F_8) - (F_8 + F_1) = \frac{1}{2} (F_{78} + F_{61}),$$

$$F_\ell = \frac{\partial F}{\partial \ell} = \frac{1}{2} (F_7 + F_3) - (F_6 + F_1) = \frac{1}{2} (F_{76} + F_{81}).$$

Then

$$|\bar{R}_k|^2 (r_k^{n+1/2})^2 + (z_k^{n+1/2})^2$$

$$|\bar{R}_\ell|^2 = (r_\ell^{n+1/2})^2 + (z_\ell^{n+1/2})^2$$

and

$$q_a = \left[\frac{\bar{R}_\ell \times \bar{U}_k}{|\bar{R}_\ell|} \right]^2 = \frac{[r_\ell^{n+1/2} v_k^{n+1/2} - r_\ell^{n+1/2} u_k^{n+1/2}]^2}{|\bar{R}_\ell|^2} = \frac{A^2}{|\bar{R}_\ell|^2} = 0 \text{ if } A < 0$$

$$q_b = \left[\frac{\bar{U}_\ell \times \bar{R}_k}{|\bar{R}_k|} \right]^2 = \frac{[z_k^{n+1/2} u_\ell^{n+1/2} - r_k^{n+1/2} v_\ell^{n+1/2}]^2}{|\bar{R}_k|^2} = \frac{B^2}{|\bar{R}_k|^2} = 0 \text{ if } B < 0.$$

The mean stress Q term is given by

$$Q_7^{n+1/2} = \rho_7^o \eta_7 \left\{ C_0^I [q_a + q_b] + C_1^I (\text{SDSP})_7 \sqrt{q_a + q_b} \right\}. \quad (\text{VII-6})$$

Notice that q_a gives the square of the velocity difference normal to the ℓ direction, while q_b gives the square of the velocity difference normal to the k direction. If the zone is expanding normal to the ℓ direction, then q_a is set to zero. If the zone is expanding normal to the k direction, then q_b is set to zero. C_0^I and C_1^I are input quantities. For most problems, values of C_0 between one and two and C_1 between 0.05 and 0.1 have succeeded in preventing oscillatory solutions.

The term containing C_0^I is analogous to the artificial viscosity first introduced by Von Neumann and Richtmyer²⁴ to permit numerical calculation of shock hydrodynamics by replacing the discontinuous pressure jump across a shock by a rapid but continuous change. The term containing C_1^I provides the damping for waves propagating at elastic velocity. In this term, the sound speed (SDSP) is given by

$$\text{SDSP} = \sqrt{\frac{\frac{dP}{dMU} + \frac{4}{3}\mu}{\rho^o}}. \quad (\text{VII-7})$$

The deviatoric tensor Q terms are

$$Q_i^{n+1/2} = C_2 (\text{SDSP})_7 \rho_7^o \eta_7 (\Delta L)_7 e_i \quad i = r, z, rz \quad (\text{VII-8})$$

where the e_i are the deviatoric strain rates given in Eq. (V-2). The factor C_2 in Eq. (VII-8) is not an independent constant, but is calculated each cycle as

$$C_2 = \frac{2\mu}{\left(\frac{dP}{dMU}\right)} C_1^I. \quad (\text{VII-9})$$

The Q_{KL_r} and Q_{KL_z} damping terms in Eqs. (III-16) and (III-17) are designed to prevent the type of zone deformation shown in Fig. 8. Since this type of deformation features equal velocities at opposite corners of a zone, then zone diagonals translate, the zone area remains constant and the strain in the zone remains constant. Therefore, no stress will develop as a result of this type of deformation.

If we consider a typical zone, say 8167 in Fig. 8, we see that the k lines 61 and 78 have opposite rotations as do the ℓ lines 76 and 81. The Q_{KL} damping terms are designed to prevent the constant strain rotations of the k and ℓ lines.

For the ℓ component of damping, we use Fig. 8a. If

$$\vec{R}_{\ell k} = \frac{\vec{R}_6 + \vec{R}_7 - (\vec{R}_1 + \vec{R}_8)}{2} = \frac{(r_{61} + r_{78}) \vec{e}_r + (z_{61} + z_{78}) \vec{e}_z}{2},$$

Fig. 8a. The f component of QKL.

Fig. 8b. The k component of QKL.

then

$$\vec{\omega}_1^k = \frac{\vec{R}_k \times (\vec{U}_6 - \vec{U}_1)}{\vec{R}_k \cdot \vec{R}_k}; \quad \vec{U}_6 = u_6 \vec{e}_r + v_6 \vec{e}_z,$$

$$\vec{\omega}_2^k = \frac{\vec{R}_k \times (\vec{U}_7 - \vec{U}_8)}{\vec{R}_k \cdot \vec{R}_k},$$

$$-\frac{\omega_2^k - \omega_1^k}{\frac{J}{|\vec{R}_k|}} = \frac{\vec{R}_k \times (\vec{U}_{61} - \vec{U}_{78})}{|\vec{R}_k| J} = -\frac{\omega_f^k}{J},$$

$$QKL_f = C_3 (SDSP) (-\vec{\omega}_f^k) \times \vec{R}_k$$

$$= \frac{C_3 (SDSP) \Omega_k [(r_{61} + r_{78})\vec{e}_z - (z_{61} + z_{78})\vec{e}_r]}{2J [(r_{61} + r_{78})^2 + (z_{61} + z_{78})^2]^{1/2}}, \quad (VII-10)$$

where $\Omega_k = (z_{61} + z_{78})(u_{16} + u_{78}) - (r_{61} + r_{78})(v_{16} + v_{78})$. For the k component of damping, we use Fig. 8b.

$$\vec{R}_f = \frac{(r_{76} + r_{81})\vec{e}_r + (z_{75} + z_{81})\vec{e}_z}{2}$$

$$\omega_1^f = \frac{\vec{R}_f \times (\vec{U}_2 - \vec{U}_1)}{|\vec{R}_f| \cdot |\vec{U}_2 - \vec{U}_1|} \quad \omega_2^f = \frac{\vec{R}_f \times (\vec{U}_7 - \vec{U}_6)}{|\vec{R}_f| \cdot |\vec{U}_7 - \vec{U}_6|}$$

$$-\frac{\omega_2^f - \omega_1^f}{|\vec{R}_f|} = -\frac{\vec{R}_f \times (\vec{U}_{16} + \vec{U}_{78})}{|\vec{R}_f|^J} = -\omega_k^f$$

$$\begin{aligned} Q\vec{K}\vec{L}_k &= C_3 \text{ (SDSP)} (-\omega_k^f) \times \vec{R}_f \\ &= \frac{C_3 \text{ (SDSP)} \Omega_f \left[(r_{76} + r_{81})\vec{e}_z - (z_{76} + z_{81})\vec{e}_r \right]}{2J \left[(r_{76} + r_{81})^2 + (z_{76} + z_{81})^2 \right]^{1/2}}, \end{aligned} \quad (\text{VII-11})$$

where $\Omega_f = (u_{16} + u_{78})(z_{76} + z_{81}) - (v_{16} + v_{78})(r_{76} + r_{81})$. If we add Eqs. (VII-10) and (VII-11) to find the $\vec{e}_r$ and $\vec{e}_z$ components, then

$$Q\vec{K}\vec{L}_f + Q\vec{K}\vec{L}_k = Q_7^r \vec{e}_r + Q_7^z \vec{e}_z$$

where

$$Q_7^r = - \left[\frac{\Omega_f (z_{76} + z_{81})}{[(r_{76} + r_{81})^2 + (z_{76} + z_{81})^2]^{1/2}} + \frac{\Omega_k (z_{61} + z_{78})}{[(r_{61} + r_{78})^2 + (z_{61} + z_{78})^2]^{1/2}} \right] \frac{\text{(SDSP)} (C_3^I)}{2J} \quad (\text{VII-12})$$

and

$$Q_7^z = \left[\frac{\Omega_f (r_{76} + r_{81})}{[(r_{76} + r_{81})^2 + (z_{76} + z_{81})^2]^{1/2}} + \frac{\Omega_k (r_{61} + r_{78})}{[(r_{61} + r_{78})^2 + (z_{61} + z_{78})^2]^{1/2}} \right] \frac{\text{(SDSP)} (C_3^I)}{2J} \quad (\text{VII-13})$$

Since the Q_7^r and Q_7^z accelerations are applied at the zone center, they are weighted with E_{61} and E_{81} combinations, like the nonderivative acceleration terms in Table 1. From Fig. 8 we see that Q_7^r , Q_7^z and Q_1^r , Q_1^z have the correct sign for damping, while Q_6^r , Q_6^z and Q_8^r , Q_8^z have the wrong sign. With these sign changes and using the weight factors of Table 1 we find

$$QKL_r = Q_7^r (1 - E_{61}) (1 - E_{81}) - Q_8^r E_{61} (1 - E_{81}) + Q_1^r E_{61} E_{81} - Q_6^r E_{81} (1 - E_{61}) \quad (VII-14)$$

and

$$QKL_z = Q_7^z (1 - E_{61}) (1 - E_{81}) - Q_8^z E_{61} (1 - E_{81}) + Q_1^z E_{61} E_{81} - Q_6^z E_{81} (1 - E_{61}) \quad (VII-15)$$

The quantity C_3^I in Eqs. (VII-12) and (VII-13) is an input constant. Values of $C_3^I \approx 0.01$ have succeeded in preventing the zone distortion of Fig. 8.

3. Δt CALCULATION

The quantity

$$N^2 = \frac{\Delta L^2}{(4C_0^I)^2 (q_a + q_b) + [1 + (2C_1^I)^2] (SDSP)} \quad (VII-16)$$

is calculated for each zone. The minimum value of N^2 determines the time step where

$$\Delta t^{n+1/2} = C_4^I \sqrt{N_{\min}^2} \quad (C_4^I \text{ is an input constant} \approx 1/2), \quad (VII-17a)$$

$$\Delta t^n = \frac{\Delta t^{n-1/2} + \Delta t^{n+1/2}}{2}, \quad (VII-17b)$$

$$t^{n+1} = t^n + \Delta t^{n+1/2}. \quad (VII-17c)$$

The stability condition given by Eqs. (VII-16) and (VII-17) is designed for both strong shocks, where $q_a + q_b$ is the dominant term in the denominator, and sonic signals, where the elastic velocity (SDSP) dominates. It is a generalization of the stability condition proposed by Von Neumann and Richtmyer²⁴ for one-dimension (plane) hydrodynamic shocks. The factor multiplying the SDSP in the denominator of Eq. (VII-16) represents the increase in elastic velocity due to the linear portion of the artificial viscosity [Eq. (VII-6)].

The code is now ready to return to Eqs. (III-16), (III-17), and (III-18) and calculate new grid point velocities (at a boundary the modified momentum equations of section IV are used). These velocities are used to increment the zone coordinates and to calculate the strain rates that correspond to the zone deformation (section V). These strain changes are related to stress changes through the equation of state (section VI). Damping terms along with the change in internal energy are calculated using the new velocities

and stresses (section VII). The stability condition of section VII [Eqs. (VII-16) and (VII-17)] is used to calculate a new time step for the entire grid. Time is incremented, and the above loop is repeated.

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