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MASTER

PHYSICS AND NUMERICS OF THE TENSOR CODE
[INCOMPLETE PRELIMINARY DOCUMENTATION]

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PREFACE

In writing this document it has been the authors' intention: to document the current state of the code and much of the thinking which has led to it; to candidly assess the shortcomings of the code and its models; and to indicate those areas which may provide profitable avenues of expansion and further study.

A great many people have contributed to the *TENSOR* code since its inception, and we have shamelessly borrowed from their writings in assembling this document. G. Maenchen and S. Sack were the originators of the code. The code described here is an offshoot of their original code, and was expanded substantially under the stewardship of J.T. Cherry who also contributed much to the fundamental constitutive models. The physics and numerics have benefitted from the ideas of T. Butkovich, R.C.Y. Chin, J. Hannon, B. Killian, J.F. Schatz, C. Snell, R. Stout, R. Swift, R. Terhune, L. Thigpen, and O. Walton. Many programmers have worked on the code and its ancillary routines: A.L. Bruce, D. Gardner, T. Kishi, V. Kransky, G. Long, J. Parlagreco, J. Shaw, and J. Owens. The code also owes much to its many users over the years and to their insatiable demands for improvements.

The development of *TENSOR* has been sponsored principally by the LLNL Containment Program in recent years. Other Department of Energy sponsors have been the Plowshare Program, Coal Program, Weapons Effects Cratering Program, as well as reimbursable work for the Department of Defense (Corps of Engineers and Defense Nuclear Agency).

The authors wish to express their appreciation to Len Margolin of Los Alamos National Laboratory and ... who were kind enough to labor through and offer their comments on this lengthy manuscript.

In an effort to provide current and timely information to code users, documentation for *TENSOR* and its ancillary routines is being computerized using LLNL text editing and graphics routines. Most of the work in this area has been done by Nancy Frary with the helpful advice of O. Walton. The following volumes of the series *TENSOR USER'S GUIDE* are planned, and most are available in at least draft form:

1. *Physics and Numerics of the TENSOR Code.*
2. *TENGEN User's Guide.*

3. *TENSOR Main Code Operating Instructions.*
4. *User's Guide to ZON: TENSOR Zoning and Service Code.*
5. *TENPLT, a Graphics, Editing, and Movie Postprocessor for Two-Dimensional Hydrocodes.*
6. *TIMPLT, an Interactive Graphics Postprocessor of TENSOR Code Time History Information.*
7. *User's Guide to SOC: Lagrangian Finite Difference Computer Code*
8. *User's Guide to ROC: an Equation of State Generator.*

While developed principally for the *TENSOR-SOC* code system, the zoning, graphics, and EOS generators are of more general utility and have been used with other code systems.

ABSTRACT

INTRODUCTION

The present *TENSOR* code is a descendant of a code originally conceived by Maenchen and Sack[3] and later adapted by Cherry[4]. Originally, the code was a two-dimensional Lagrangian explicit finite difference code which solved the equations of continuum mechanics. Since then, implicit[5] and arbitrary Lagrange-Euler (ALE)[6] algorithms have been added. The code has been used principally to solve problems involving the propagation of stress waves through earth materials, and considerable development of rock and soil constitutive relations has been done[77,78,71,33]. The code has been applied extensively to the containment of underground nuclear tests[59, 1], nuclear and high explosive surface[2] and subsurface[83,84,85] cratering, and energy and resource recovery[86,87].

In its current configuration, a problem of about 10,000 zones will run core contained on a CDC 7600 computer using about 95% of core. Larger problems may be run using worker disks but with lower efficiency. Recent problems show a computational rate of roughly 2000 zone-cycles/CPU-sec. The current code carries 26 words of storage per zone containing about 35 physics variables. Conversion to the CRAY computer is presently underway.

TENSOR is supported by a substantial array of ancillary routines. The initial conditions are set up by a generator code *TENGGEN*. *ZON* is a multipurpose code which can be used for zoning, rezoning, overlaying, and linking from other codes. Linking from some codes is facilitated by another code *RADTEN*. *TENPLT* is a fixed time graphics code which provides a wide variety of plotting options and output devices, and which is capable of producing computer movies by postprocessing problem dumps. Time history graphics are provided by the *TIMPLT* code from temporal dumps produced during production runs. While *TENSOR* can be run as a stand-alone controllee, a special controller code *TCON* is available to better interface the code with the LLNL computer system during production jobs. In order to standardize compilation procedures and provide quality control, a special compiler code *BC* is used. A number of equation of state generators are available among them *ROC* and *PMUGEN*.

Formulation

Although *TENSOR* can be used in either plane or cylindrical coordinates (r, z, θ) , the latter mode is most often used, and consequently, will be the one described here. The appropriate equations for plane-strain can be obtained by considering the limit of large r . The region to be described in the calculation is discretized into a large number of quadrilateral zones in the r - z plane, the z -axis being the symmetry axis.

The state of the material within each zone is described by a stress tensor (σ) and a strain tensor (ε) which are both separated into their isotropic (P and Θ) and deviatoric (S and e) components,

$$\begin{bmatrix} \sigma_r & \sigma_{rz} & 0 \\ \sigma_{rz} & \sigma_z & 0 \\ 0 & 0 & \sigma_\theta \end{bmatrix} = -P\mathbf{I} + \begin{bmatrix} S_r & S_{rz} & 0 \\ S_{rz} & S_z & 0 \\ 0 & 0 & S_\theta \end{bmatrix} \quad (1)$$

$$\begin{bmatrix} \varepsilon_r & \varepsilon_{rz} & 0 \\ \varepsilon_{rz} & \varepsilon_z & 0 \\ 0 & 0 & \varepsilon_\theta \end{bmatrix} = \frac{\Theta}{3}\mathbf{I} + \begin{bmatrix} e_r & e_{rz} & 0 \\ e_{rz} & e_z & 0 \\ 0 & 0 & e_\theta \end{bmatrix}$$

where $\mathbf{I}$ is the identity tensor. The pressure or mean stress P and the volumetric strain Θ are then given by:

$$P = -\frac{1}{3}(\sigma_r + \sigma_z + \sigma_\theta)$$

$$\Theta = \varepsilon_r + \varepsilon_z + \varepsilon_\theta.$$
(2)

The introduction of the first invariant quantities, P and Θ , allows the θ components to be carried implicitly in the solution. The off-diagonal

components, σ_{rz} and S_{rz} , are of course identical, as are ϵ_{rz} and e_{rz} . For historical reasons, the sign conventions are such that stress and strain are positive in tension and extension respectively; while pressure is positive in compression.

Conservation of momentum is expressed as,

$$\rho \dot{\mathbf{u}} = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g} \quad (3)$$

In terms of P and the deviatoric stresses, the conservation laws reduce in cylindrical coordinates to the coupled equations of motion,

$$\begin{aligned} \rho \dot{u} &= -\frac{\partial}{\partial r}(P - S_r) + \frac{\partial}{\partial z}S_{rz} + \frac{1}{r}(2S_r + S_z) + \rho g_r \\ \rho \dot{v} &= -\frac{\partial}{\partial z}(P - S_z) + \frac{\partial}{\partial r}S_{rz} + \frac{1}{r}S_{rz} + \rho g_z. \end{aligned} \quad (4)$$

where u is the velocity, ρ is the density, and g is the gravitational body acceleration. Dissipative viscosity terms which are added to each of the stresses to smooth the sharp discontinuities characteristic of shock phenomena are not shown in the above equations.

The accelerations are integrated to yield the velocities, u and v and the new coordinates, r and z . From geometrical considerations, the strain rates can then be calculated as,

$$\begin{aligned} \dot{\theta} &= \frac{\partial}{\partial r}u + \frac{\partial}{\partial z}v + \frac{u}{r} \\ \dot{e}_r &= \frac{1}{3}\left(2\frac{\partial}{\partial r}u - \frac{\partial}{\partial z}v - \frac{u}{r}\right) \\ \dot{e}_z &= \frac{1}{3}\left(2\frac{\partial}{\partial r}v - \frac{\partial}{\partial z}u - \frac{u}{r}\right) \\ \dot{e}_{rz} &= \frac{1}{2}\left(\frac{\partial}{\partial r}v + \frac{\partial}{\partial z}u\right). \end{aligned} \quad (5)$$

The resulting strain rates are then used to calculate the stress rates and consequently the new stresses. During each code cycle, stress loading is treated initially as an incrementally elastic or "hypoelastic"[68] process which can be described by two independent elastic moduli over the range of

stresses encountered during a single time step. The calculated stresses are later adjusted, as necessary, to take into account any inelastic behavior as described by the constitutive model.

Temporal Discretization

Figure 1 illustrates the temporal discretization employed in integrating the above differential equations. The procedure used here constitutes an explicit central difference method. An implicit scheme is described in a later section.

Figure 1. Explicit Calculation Procedure

The first step in the calculational cycle is to advance zone centered variables, an operation which is done within one subroutine. Velocities and coordinates at $n-1/2$ are used to calculate strain rates which are combined with material moduli to advance stress σ from $n-1$ to n . For reasons to be discussed later, artificial viscosities Q are calculated at $n-1/2$ but are used as if centered at n . The internal energy deposition rate $\dot{E}$ is then calculated to advance internal energy E from $n-1$ to n . For energy-dependent

constitutive relations an iteration is done to arrive at the final stress and internal energy.

Operations on nodal variables are done in another subroutine. As with artificial viscosity, the hourglass viscosities are calculated at $n-1/2$ but used at n . Stress gradients at n are used to calculate acceleration at n . This is then used to advance velocity u from $n-1/2$ to $n+1/2$. This in turn advances displacements and coordinates from n to $n+1$.

CONSTITUTIVE MODELING

While the constitutive models in the *TENSOR* code have been developed principally for earth sciences applications, most of the model features are generally applicable to other materials. The qualitative thinking implicit in the *TENSOR* failure models is analogous to but less detailed than that of some of the statistical micromechanical models currently being developed [40,41,42,43,44, 45,46,47]. The lack of detail is compensated by the applicability of the model to loading conditions more general than those normally addressed by such models. In many cases, statistical models can be made to conform to the *TENSOR* forms by the substitution of appropriate expressions for damage, relaxation times, and so forth.

Elasticity

For elastic constitutive relations, stress rates and strain rates are related by a matrix of elastic constants **D**. With

$$\begin{aligned}\sigma &= \{\sigma_r, \sigma_z, \sigma_\theta, \tau_{rz}\}^{-1} \\ \varepsilon &= \{\varepsilon_r, \varepsilon_z, \varepsilon_\theta, \gamma_{rz}\}^{-1} \\ \dot{\sigma} &= \mathbf{D} \dot{\varepsilon}\end{aligned}\tag{6}$$

and

$$\mathbf{D} = \begin{bmatrix} \lambda+2G & \lambda & \lambda & 0 \\ \lambda & \lambda+2G & \lambda & 0 \\ \lambda & \lambda & \lambda+2G & 0 \\ 0 & 0 & 0 & G \end{bmatrix}\tag{7}$$

$$\mathbf{D}^{-1} = \frac{1}{E} \begin{bmatrix} 1 & -\nu & -\nu & 0 \\ -\nu & 1 & -\nu & 0 \\ -\nu & -\nu & 1 & 0 \\ 0 & 0 & 0 & \frac{E}{G} \end{bmatrix}$$

The fundamental pair of elastic constants are taken to be the bulk modulus k and Poisson's ratio ν . In terms of them the shear modulus G , Young's modulus, and the Lamé modulus are given by

$$G = \frac{3k}{2} \left(\frac{1 - 2\nu}{1 + \nu} \right)$$

$$E = 3k(1 - 2\nu)$$

$$\lambda = \frac{3k\nu}{1 + \nu}$$

Later sections describe the model assumed in determining the bulk modulus and in the integration of the deviatoric equations. Briefly, the model uses an elastic bulk modulus k and an elastic shear modulus G which are characteristic of the current state of the material. Linearity of the moduli during the load increment is not assumed. This is a "variable modulus" model in that it assumes a pressure dependent k and a similar dependence in G if a constant Poisson's ratio (ν) is assigned. The shear modulus can optionally be constrained not to exceed a limiting value $G_{\max}$. In addition, the bulk modulus may also depend on the previous state of the material, as discussed below.

Expressions for fluids are obtained as a special case by setting the shear modulus to zero. The modeling of gradual phase transitions between the solid and fluid state is achieved through the artifice of using an effective shear modulus,

$$G = \begin{cases} G_0 & E_f < 0 \\ G_0 \left(1 - \frac{E}{E_f} \right) & 0 \leq E \leq e_f \\ 0 & E > E_f \end{cases}$$

where G_0 is the shear modulus for the solid, E_f is the specific internal energy of fusion, and E is the current specific internal energy.

Inelasticity

The total strain rate is a sum of geometrical rate $\dot{\epsilon}$ and a pseudo-strain rate $\dot{\epsilon}^G$ due to heating (e.g., a Gruncisen form). In inelastic continuum mechanics, one fundamental assumption is that the total strain rate $\dot{\epsilon}$ can be expressed as the sum of elastic $\dot{\epsilon}^E$ and inelastic $\dot{\epsilon}^P$ components. This corresponds to the notion that the applied strain is picked up by both the material matrix and the inelastic discontinuities within the matrix. This assumption forms the foundation of the failure models described below. Such a decomposition is strictly valid only if the elastic strains are infinitesimal [60,61]. This suggests the need for a timestep constraint which is often ignored in practice, since the Courant-Friedrichs-Lewy (CFL) limit [7, 8] is usually sufficient. The inelastic strain rate can in turn be broken into parts corresponding to various inelastic processes: pore collapse, ductile and brittle shear failure, tensile failure and void formation, and void closure.

$$\begin{aligned}\dot{\epsilon} + \dot{\epsilon}^G &= \dot{\epsilon}^E + \dot{\epsilon}^P \\ &= \dot{\epsilon}^E + [\dot{\epsilon}^C + \dot{\epsilon}^S + \dot{\pi}]\end{aligned}\quad (8)$$

in which $\dot{\epsilon}^C$ is the plastic volume strain rate resulting from the collapse of homogeneously distributed pores and is diagonal; $\dot{\epsilon}^S$ is the plastic shear strain rate resulting from shear failure and has zero trace; and $\dot{\pi}$ is the void strain rate which results from tensile failure.

For inelastic constitutive relations, it is the elastic contribution to the stress rate which must be solved for. Expressed in incremental form, the decomposition (Equation 8) can then be thought of as an elastic stress increment followed by an inelastic stress relaxation.

$$\begin{aligned}\sigma^{n+1} &= \sigma^n + D \dot{\epsilon}^E \delta t \\ &= [\sigma^n + D(\dot{\epsilon} + \dot{\epsilon}^G) \delta t] - D(\dot{\epsilon}^C + \dot{\epsilon}^S + \dot{\pi}) \delta t \\ &= \tilde{\sigma}^{n+1} - \Delta \sigma^C - \Delta \sigma^S - \Delta \sigma^T\end{aligned}\quad (9)$$

in which $\tilde{\sigma}$ is a trial stress based upon the total strain rate and the $\Delta \sigma$ are inelastic stress adjustments determined by the failure flow rules. Given the stress adjustments, the corresponding plastic strains are determined from Equation 6. The failure flow rules fall into three principal

categories: pore collapse, shear failure, and tensile failure. The flow relations for these processes are coupled in the sense that they each place separate constraints on the stress components. In principle, they form a system of equations which should be solved simultaneously either directly or by iteration. However, by following the hierarchy described below, a single pass has been sufficient for current code applications.

For simplicity, the tilde $\sim$ indicating trial values will be dropped in the following. In the r - z representation, the trial isotropic and deviatoric stress rates are given by,

$$\dot{p} = -k\dot{\theta}$$

$$\dot{S}_r = 2G\dot{e}_r + 2S_{rz}\omega_{rz} \quad (10)$$

$$\dot{S}_z = 2G\dot{e}_z - 2S_{rz}\omega_{rz}$$

$$\dot{S}_{rz} = 2G\dot{e}_{rz} + (S_z - S_r)\omega_{rz},$$

where the factor

$$\omega_{rz} = \frac{1}{2}\left(\frac{\partial u_r}{\partial z} - \frac{\partial u_z}{\partial r}\right) \quad (11)$$

is an angular velocity which corrects for the rigid body motion of the zone during the time step. The above is the so-called Jaumann definition of stress rate [88]. The finite difference equations actually used in the code carry an additional higher order rotation term not shown in the above differential equations.[89]

Tensor Rotational Properties

We briefly describe the Mohr circle and the coordinate transformations of the stress and strain tensors. We refer the reader to Jaeger[48] and the historical work of Mohr [49,60] for further detail. To represent a stress

tensor in a Mohr diagram, one plots the principal stresses along a horizontal axis and shear stress along the vertical. A circle centered on the horizontal axis is then drawn through the two principal stress points as shown in Figure 2. Consider a plane whose normal is at an angle 2θ from the z axis (Figure 3). The normal stress σ and shear stress τ can be readily determined from the Mohr diagram. A line drawn at an angle 2θ intersects the circle at the point (σ, τ) .

Figure 2. Mohr circle representation of the stress tensor.

Figure 3. Relative orientation of the shear plane.

This result allows us to easily write expressions for the principal stresses in terms of the r - z components. Suppose that σ and τ are the σ_z and σ_{rz} components of the stress tensor in the r - z system. In our convention the angle θ is always measured from the z axis. Then from Figure 2, the principal stresses are simply

$$\left. \begin{matrix} \sigma_2 \\ \sigma_1 \end{matrix} \right\} = \frac{1}{2}(\sigma_r + \sigma_z) \pm [\sigma_{rz}^2 + \frac{1}{4}(\sigma_z - \sigma_r)^2]^{1/2} \quad (12)$$

and

$$\tan 2\theta = \frac{2\sigma_{rz}}{\sigma_z - \sigma_r} \quad (13)$$

$$\begin{aligned} \sin 2\theta &= \frac{\sigma_{rz}}{[\sigma_{rz}^2 + \frac{1}{4}(\sigma_z - \sigma_r)^2]^{1/2}} \\ &= 2\sin\theta\cos\theta \end{aligned}$$

$$\begin{aligned} \cos 2\theta &= \frac{\frac{1}{2}(\sigma_z - \sigma_r)}{[\sigma_{rz}^2 + \frac{1}{4}(\sigma_z - \sigma_r)^2]^{1/2}} \\ &= \begin{cases} 1 - 2\sin^2\theta \\ 2\cos^2\theta - 1 \end{cases} \end{aligned}$$

In the above equations θ is the angle of rotation from the r-z system to a system in which the tensor is diagonal. Similarly, by considering Figure 4, the results of any rotation through angle φ can be derived,

$$\begin{aligned} \sigma'_r &= \sigma_r \sin^2\varphi + \sigma_z \cos^2\varphi + 2\sigma_{rz} \sin\varphi \cos\varphi \\ \sigma'_z &= \sigma_r \cos^2\varphi + \sigma_z \sin^2\varphi - 2\sigma_{rz} \sin\varphi \cos\varphi \\ \sigma'_{rz} &= (\sigma_r - \sigma_z) \sin\varphi \cos\varphi + \sigma_{rz} (\cos^2\varphi - \sin^2\varphi) \end{aligned} \quad (14)$$

Figure 4. Rotation of stress tensor
in Mohr circle representation.

Pressure Integration

In general, the pressure will be a function of both internal energy and specific volume. Fluid models in *TENSOR* take this energy dependence into account by analytical forms, such as the Tillotson^[57] form and the Jenkins-Wilkins-Lee (JWL)^[58] form for explosive detonation products. Energy dependence in rock and soil constitutive relations is accounted for either by an adiabatic release path formulation^[34,35] or by a Gruneisen^[55,56] form.

The model used in determining the effective bulk modulus for earth materials takes into account two effects. The first is the permanent loss of porosity which occurs as the strength of the material bonds is exceeded. The second is the void volume which is produced concomitant to tensile failure.

In practice, there are two distinct ways to carry out the pressure integration. In the first method, the compression η is integrated directly, and P is determined as a function of η (or the excess compression μ) and other appropriate parameters.

$$\eta = \rho/\rho_0$$

$$\mu = \eta - 1$$

$$= -\eta \int \dot{\epsilon} dt \quad (15)$$

$$P = P(\mu, \dots)$$

So long as the function $P(\mu, \dots)$ is sufficiently general to describe the complete state of the system, this method can be used. However, as presently formulated, dilatational flow rules such as those resulting from tensile failure will cause the material to be adjusted away from this functional value. Once this happens, this form of integration can no longer be used because the pressure could change discontinuously between cycles.

In the second method, the bulk modulus is determined as a function of P or μ , and P is then integrated directly. However, as indicated above, the presence of dilatational flow values can cause large errors if the modulus is taken to be a function of μ . For this reason, the following form is used,

$$\begin{aligned} k(P) &= \eta \frac{\partial P}{\partial \mu} \\ &= \eta \alpha(P, \dots) \end{aligned} \quad (16)$$

$$\begin{aligned} P &= \int k(P) d\mu / \eta \\ &= \int \alpha(P, \dots) d\mu \end{aligned}$$

where α is the slope of the current trajectory in P - μ space. The slope method has the advantage of producing a very robust algorithm which seldom runs into numerical difficulties. Since α is expressed as a function of P a special procedure is needed to avoid improperly centering α at $n-1$ rather than $n-1/2$, constituting a forward rather than central difference. This deficiency is corrected in the code by calculating an effective $\mu_e(P^{n-1})$, the trial pressure. $P_t^n(\mu_e + \delta\mu)$, and then $\alpha^{n-1/2} = (P_t^n - P^{n-1})/\delta\mu$. The trial pressure will turn out to be the final pressure if no failure processes occur.

Pore Collapse

Pore collapse is modelled by a procedure^[70,71] which is analogous to the well-known P - α model^[51,52,53]. While not expressed in these terms, the following description of pore collapse can be thought of as described in Equation 9, that is, as an elastic loading with a modulus characteristic of fully compacted material, followed by a plastic volumetric strain in which pores close and pressure is relaxed to a lower level. The collapse of intrinsic pores and cracks is modeled by including the maximum pressure P_x in the functional relationship,

$$P = P(\mu, P_x) \quad (17)$$

A given material is assumed to be describable in terms of two pressure-volume relationships, such as those labeled A and B in Figure 5. These relations are given to the code as tables of pressure versus the excess compression μ . A number of empirical schemes are available for generating these curves for common materials ^[36,37,38].

The prescription followed in determining α , and therefore k , is illustrated in Figure 5. The material is taken to load along a path termed the virgin loading path (A). When porous flow is calculated explicitly in the code, this curve should represent the results of "fully drained" hydrostatic or uniaxial loading laboratory tests in which the sample is unsealed and the loading is sufficiently slow that pore fluid is free to flow through the sample. When pore fluid effects are not treated explicitly, this curve should implicitly incorporate these effects and this should represent the result of an "undrained" test. In this section pores will be considered to be filled with vacuum, pore fluid effects being considered later.

Subsequent unloading behavior depends on the maximum compression P_x experienced by the material relative to two experimental points P_1 and P_2 . If P_x has not exceeded P_1 , then no permanent compaction can take place because the internal stresses have not exceeded the pore wall strength and allowed pore collapse to occur. Examination of compressibility data for a number of rocks indicates that the threshold pressure P_1 for pore collapse is dependent upon the shear strength, the air-filled porosity, and also the water content^[36,39]. In practice, the slope of curve A between the origin and P_1 is usually selected to yield the correct sonic velocity for low amplitude signals. In matching low amplitude signals, it may be necessary to use a more gradual transition in slope in the vicinity of P_1 than indicated in Figure 5.

Figure 5: Pressure Volume Model.

Above P_2 which can be arbitrarily high, curves A and B are presumed to coincide. If the maximum pressure P_x has exceeded P_2 , then all pores have presumably collapsed; and the material must unload along the path B for completely crushed material. When pore fluid effects are explicitly considered, the crushed path should be the unloading path for pure nonporous matrix material. When pore fluid effects are not explicitly considered, they should be imposed implicitly in the crushed path. The intercept μ_3 is the maximum permanent compaction and is approximately equal to the porosity of the material ($\phi = \mu_3/\eta_3$).

When P_x is greater than P_1 but does not yet exceed P_2 , then the material is only partially compacted and must unload along a path between the crushed and virgin loading curves. If the partial pore collapse were permanent, the appropriate unloading path would have to be consistent with the unloading behavior of the fully crushed matrix material. That is to say, partially crushed material would have to unload along path C in Figure 5, which is parallel to the crushed path B and will intersect the μ axis at μ_r .

$$\mu_r^*(\mu_x) = \mu_3 - (\mu_B - \mu_x).$$

in which μ_x is the excess compression corresponding to P_x .

However, partially compacted material usually exhibits elastic recovery of some porosity, presumably because many of the pore walls have not been stressed to failure. This means that the material must unload along some path D which lies to the left of C. The specification of this path is accomplished as follows. The residual porosity, which is the intercept μ_r of D with the μ axis, can be deduced from laboratory data and expressed as a polynomial,

$$\mu_r(\mu_x) = \mu_3(A_1s + A_2s^2 + A_3s^3) \quad \mu_1 \leq \mu_x \leq \mu_2, \quad (18)$$

where the sum of the A_i coefficients must be unity to guarantee that $\mu_r(\mu_2) = \mu_3$. The quantity s is related to the maximum compression and is expressed as a fraction,

$$s(\mu_x) = \frac{\mu_x - \mu_1}{\mu_2 - \mu_1} \leq 1. \quad (19)$$

It is then necessary to require that D lie to the left of C and intersect the μ axis at μ_r . If the recovered porosity ($\mu_r^* - \mu_r$) is assumed to be restored as a linear function of P , then the following relationship for α along path D is easily derivable,

$$\frac{1}{\alpha(P)} = \frac{1}{\alpha_c(P)} + \frac{\mu_r^* - \mu_r}{P_x}, \quad (20)$$

where α_c is the slope of C at pressure P . Since α is determined, the effective bulk modulus k is known and the pressure integration can be accomplished. Infinite or negative slopes are not forbidden by Equation 20. Should such a value be calculated, it is replaced by the slope of a straight line drawn between μ_x and μ_r . Although setting the slope to α_c might seem to be more appropriate, such a procedure could cause unintentional bulking by unloading to the left of the origin, depending on the shape of path B.

Rate Dependence

At present there is no explicit treatment of viscous pore collapse in *TENSOR*. Such a treatment would involve the addition of a strain-rate dependent term to the pressure relation. Models for this effect have been developed^[64] and could be incorporated with little effort. Mathematically, this form is a Voigt relaxation and is analogous to the form of the artificial viscosity. In a later section, a special Q is developed to remove noise associated with the rapid collapse of porous material on artificial viscosity. With proper normalization to material properties rather than numerical properties, this form could be used to treat viscous pore collapse. Particular attention must be paid to the stability criterion in any of these methods.

Overburden Correction

The user has the option to include the gravitational terms. When they are included, each zone is given an initial overburden pressure which balances the equations of motion and produces an initial equilibrium. Stress deviators can also be initialized to account for tectonic stresses.

Implementation leads to problems for porous materials. Suppose that at a given depth, the overburden pressure exceeds P_1 the threshold pressure for pore collapse. Below this depth, pore collapse would begin to occur as soon as a calculation is started, a completely unrealistic result. Further, at depths below which the overburden is P_2 no porosity can be sustained. If left uncorrected, very unusual wave propagation would be calculated in problems which span a large range of depths.

A key question is how geologic material is typically emplaced. Certainly it has not been emplaced like an elastic solid and then loaded over the entire depth of the problem. Geologically, such material is normally emplaced in layers in a porous state. The material either has shear strength initially or develops it through cementation over geologic time. The threshold for pore collapse P_1 which is related to the shear strength is then relatively independent of depth.

In *TENSOR* this problem is solved by giving material at each depth a slightly different constitutive relation. The origin of P - μ space is offset by the initial conditions of P_0 and μ_0 . Thus, the pressure must increase by an amount P_1 above its initial P_0 value at each depth before pore collapse can occur. The overburden pressure P_0 is carried as a constant for each zone in the calculational grid.

Associated Flow Rules

A number of models have been developed to couple shear and volumetric behaviour by means of associated flow rules in which the flow behavior is related to the shape of some yield surface. Examples are the Cap[...], Cam clay[...], and Putah Petra[...] models. These models can be used to model such behavior as shear-enhanced compaction and compaction hardening of porous materials as well as dilatant behavior during compression.

Aside from the indirect user-provided coupling introduced by the choice of the toe P_1 and merge point P_2 in the virgin loading curve, there is presently no coupling in *TENSOR* between the shear and pore collapse models. With present models, dilatancy occurs during tensile failure but not during compressive shear failure. A model for the latter along the lines of References 61 and 62 will be considered at a later date.

Pore Fluid Effects

[To be described at a later date.]

Other Forms

Gruneisen.

Jenkins-Wilkins-Lee.

Tillotson.

Explosive Burn.

Shear Failure

The modeling of shear failure as discussed below is basically a modified elastic-plastic model. The code employs both ductile and brittle modes of shear failure, the former being a special case of the latter. For ductile shear failure (yielding), the deviatoric state of the material is constrained not to exceed some yield surface which is a function of stress tensor invariants. Rate effects are incorporated by allowing the state to overshoot the yield surface and then relax back toward it with a characteristic Maxwell relaxation time.[76]

For brittle shear failure, the yield surface softens, decreasing with increasing material "damage," a quantity which will be defined later and which is related to the amount of inelastic strain.

In general, the failure surfaces are functions of stress tensor invariants[76] corresponding to the assumption that the shear properties of the matrix material are isotropic. In terms of the stress deviators, three such invariants are:

$$P = -J_1/3 = -\frac{1}{3}(\sigma_r + \sigma_z + \sigma_\theta)$$

$$J'_2 = S_r^2 + S_z^2 + S_r S_z + S_{rz}^2 \quad (21)$$

$$J'_3 = (S_r + S_z)(S_{rz}^2 - S_r S_z)$$

Data for rock materials indicates that the ductile failure surface can often be adequately described in terms of P and J'_2 alone or equivalently P and Y which is defined to be

$$Y = \left(\frac{3}{4} J'_2\right)^{1/2} \quad (22)$$

Y is proportional to the octahedral shear stress and is equal to the maximum shear stress $|\sigma_1 - \sigma_2|/2$ under uniaxial loading ($\sigma_2 = \sigma_3$).

In the realm of brittle failure (which occurs at lower pressures than ductile failure), compression, extension, and torsion data often cannot be reconciled into a single failure surface by employing only two of the invariants.[78,79] However, the data can often be reduced to a single surface defined in terms of Y and the quantity,

$$\bar{P} = P - \left(\frac{J'_3}{16} \right)^{1/3}, \quad (23)$$

which reduces to $\bar{P} = P + Y/3 = |\sigma_1 + \sigma_2|/2$ for uniaxial strain ($\sigma_2 = \sigma_3$). In the ductile region, the second term is negligible, so that both brittle and ductile failure surfaces will be described in terms of only Y and $\bar{P}$.

In the section on tensile failure a scheme is described in which the maximum shear stress between pairs of principal stresses is used to describe failure rather than the rotational invariant Y . In effect, the Mohr circle for each pair of principal stresses is compared with the shear failure criterion. This involves three tests rather than one, but such a procedure is probably more realistic when brittle failure is involved. Eventually, we anticipate that this type of algorithm may replace the one described here.

Yield Surfaces

The shape of the failure surfaces is similar to that of a modified Prager-Drucker yield criterion.[74,73] Under uniaxial loading, this yield criterion amounts to pinning the maximum shear stress (the peak of a Mohr circle) to the yield surface. This is equivalent to the commonly used Mohr-Coulomb criterion[48] in which the Mohr circle is forced to be tangent to a different yield surface which is derivable from this one. If the yield surface is horizontal, it is termed a Von Mises type. If the surface increases with pressure, a form of pressure hardening has been introduced.

The concept of brittle failure or strain softening employed in *TENSOR* is depicted in Figure 6 and assumes that the strength of virgin (unfailed) material can be characterized by a curve Y_v in Y - $\bar{P}$ space which can be defined by laboratory data, usually triaxial. The unconfined compression test, for example, will define one point along a 45 degree line from the origin. If the material has tensile strength, Y_v will intersect the $\bar{P}$ axis at a negative value of $\bar{P}$.

Material that has failed in the brittle mode is assumed to strain

soften and to be characterized by a lower strength envelope Y^e that depends on the amount of damage the material has undergone. The damage ϵ^D is defined on page 36 and is somewhat analogous to the plastic strain $J_2'(\epsilon^P)$. In particular, it is assumed that for some limiting value ϵ_{0s}^D of the damage parameter, the material has completely failed. It will then possess its lowest possible strength Y_f which arises only from the interlocking of the fragments under pressure. Such a material would possess no cohesive or equivalently tensile strength, and Y_f should pass through the origin. (However, the user should note the consequences of doing this described below.)

A final constraint on Y_v , Y , and Y_f is that they just join at the transition ($\bar{P}_{bd}$) into the ductile region, in effect requiring that there be no sharp discontinuity in the strength descriptions between the brittle and ductile regions. Figure 6 depicts curves satisfying these constraints.

In terms of Y_v and Y_f , the location of the effective failure surface at a given $\bar{P}$ is taken to be

$$y^e(\epsilon^D) = \begin{cases} Y_v - (Y_v - Y_f) \epsilon^D / \epsilon_{0s}^D & \epsilon^D < \epsilon_{0s}^D \\ Y_f & \epsilon^D \geq \epsilon_{0s}^D \end{cases} \quad (24)$$

where all quantities are to be evaluated at $\bar{P}$. This form assumes that the effective failure surface is a linear function of a scalar damage parameter ϵ^D . Other forms which allow a more gradual onset or termination could certainly be justified.

In specifying yield surfaces, code users should devote particular attention to the interaction of the shear and tensile modes of failure. States to the left of the unity slope line have at least one principal stress in tension and behavior in this region is dominated by the tensile failure algorithm. The intersections of the yield surfaces with the unity slope line correspond to the so-called "unconfined compression" states often measured in laboratory experiments. In crossing this line the mode of material failure changes from diagonal shear fracturing on the right to parallel tensile fracturing to the left. Even badly fractured material usually has some cohesion, and the common practice of passing the yield surface through the origin (*i.e.*, zero cohesion) is inappropriate unless truly fluid behavior is desired. This can be seen from the following argument. If the material is being forced into extension and consequently tensile failure, then there will be open voids. Such loading is

Figure 6. Shear Failure Surfaces.

characteristic of surface material in cratering problems. As explained later, the boundary condition on open voids will force one point on the Mohr circle to the origin. As the only Mohr circle satisfying both this condition and a zero cohesion yield surface is one of zero radius centered at the origin, the coupling of the two conditions forces a state of zero shear stress and consequently fluid behavior.

Work or strain hardening^[89] is simply accomplished by multiplying the effective strength Y^e by the factor

$$[1 + C_1 \epsilon^D]^{C_2}$$

in which C_1 and C_2 are chosen for the particular material. Compaction hardening due to the interlocking of grains during pore collapse is not presently considered, but could be with minimal effort.

Shear Flow Rule

In $Y-\bar{P}$ space, material which is shocked will load along a path of slope approximately $(1-2\nu)$, corresponding to uniaxial strain loading. Let us suppose that the integration of the incrementally elastic problem Equation 10 gave solutions $\hat{S}_r$, $\hat{S}_z$, and $\hat{S}_{rz}$ which in turn gave a value $\hat{Y}$ which lies above the failure surface Y^e at some $\bar{P}$. Next, it is necessary to prescribe how the deviatoric stresses are to be relaxed in relation to the effective failure surface Y^e . One option is to simply "pin" the material to Y^e . We, however, use a viscoelastic model, which allows some rate dependence to be

taken into account. The model used for brittle failure is that of a simple Maxwell solid in shear. In effect, this means that stress adjustment behaves as a viscous term in the stress rate Equation 10. The form used in the code is

$$S_i = \begin{cases} \tilde{S}_i [1 - \frac{\delta t}{\tau} (1 - Y^e/Y)] & \tilde{Y} > Y^e \\ \tilde{S}_i & \tilde{Y} \leq Y^e \end{cases} \quad (i = r, z, rz), \quad (25)$$

where δt is the time step. This model produces a damping which increases as $\tilde{Y}$ exceeds Y^e , and which is zero when $\tilde{Y}$ and Y^e coincide. The quantity τ , called the Maxwell relaxation time, is the characteristic time over which the stress relaxation is to take place.

In statistical fracture models, rate effects arise naturally through the time required for fracture propagation to occur. In the limit of complete fragmentation, one would expect no rate effects to be observed. Accordingly, τ can be related to the damage in such a way that $\tau \rightarrow 0$ as $\epsilon^d \rightarrow \epsilon_0^d$.

It should be noted that if τ is taken to be δt , then the state is pinned to the yield surface. As an option, the relaxation can be disabled in the ductile region through an artifice which allows the unified treatment of both brittle and ductile relaxation. This is accomplished by defining,

$$\tau = \text{Max}\{\tau_0 [1 - Y_f/Y_v], \delta t\} \quad (26)$$

where τ_0 is the input relaxation time. This relation produces an effective relaxation time which reduces to δt in the ductile region, which is τ_0 when $Y_f = 0$, and which possesses a smooth transition between the two limits.

The net effect of Equation 26 is to allow Y to overshoot the failure surface Y^e in the brittle region under rapid loading conditions (thus producing a "rate hardening"), and to gradually force the overshoot to vanish as the ductile transition is approached. This is done in the interest of using an elastic-perfectly plastic model of ductile flow. It may well be that rate dependence in the ductile region is also desirable, in which case Equation 26 should be modified or discarded.

Tensile Failure

A complete description of tensile failure involves much more than the simple relaxation of the tensile stresses. It must also describe all subsequent behavior (*via* flow rules) resulting from the boundary conditions imposed by the fractures themselves. The *TENSOR* formulation is based upon several tensor quantities: (1) the stress tensor σ , (2) the void strain tensor π , (3) the plastic shear strain tensor ϵ^S , and the strength tensor T . The role of the stress tensor is obvious; it is the stresses which must be adjusted to match the boundary conditions.

The void strain tensor π serves as a directional accounting device which keeps track of the size and orientation of the tension produced fractures, and can be thought of as a moment of some statistical crack distribution. The use of a full tensor to describe the void strain is a generalization of several other formulations [72,81] which describe the behavior of individual cracks, and reduces to them when the π tensor has only one principal component. The current formulation allows cracks to form simultaneously in each of the principal stress directions, a situation which is commonly encountered. Furthermore, the principal crack orientation can change when material which has been minimally failed is reloaded in another direction. This is the proper behavior for failure processes which can be thought of as the coalescence of microfractures.

Conceptually, tension induced voids differ from porosity in several ways. Porosity is imagined to be isotropic and to possess some resistance to closure. Tensile voids are imagined to be divided cracks which have negligible resistance. When porous flow is considered, the pore fluid is assumed to penetrate both types of voids.

The plastic shear strain tensor ϵ^S and the void tensor serve to describe the extent of damage to the material in a manner to be described later.

The material is assumed to be characterized by a virgin strength tensor T^0 . The tensor character is necessary in order to describe strength properties of layered materials. The effective tensile strength of a given zone of material is related to the virgin strength as follows:

$$T^e = \begin{cases} T^o (1 - \varepsilon^D / \varepsilon_{oT}^D) & \varepsilon^D < \varepsilon_{oT}^D \\ 0 & \varepsilon^D \geq \varepsilon_{oT}^D \end{cases} \quad (27)$$

in which ε^D is the scalar damage the zone has undergone; ε^D will be defined explicitly later. The notion here is that microcracks form in the material as the virgin strength is exceeded, causing the material to strain inelastically. As the material is strained, microcracks coalesce to form macroscopic fractures thereby reducing the ability of the material to support tension. As ε^D approaches a limiting value of ε_{oT}^D , the tensile strength becomes zero, corresponding to complete failure. Empirically this happens at damage levels of 10^{-3} to 10^{-2} . [80,78]

Principal System

While shear failure is formulated in terms of stress tensor invariants, tensile failure takes place with respect to the coordinate system of either the principal stresses or the principal void strains and consequently is formulated in terms of components in one of these systems. For small damage levels, ($\varepsilon^D \leq \varepsilon_{oT}^D$) the material is said to be in the nucleation and growth[...] phase in which the sites of failure are local and the material has no global memory of the orientation of past failure. In this phase, strength, stress, and void tensors are all rotated to the principal coordinate system of the stress tensor as indicated in Equations 13 and 14.

For large damage levels, ($\varepsilon^D > \varepsilon_{oT}^D$) the material is said to be in the fragmentation phase, the microcracks are considered to have coalesced, and the relaxation must take place in the principal coordinate system of the void tensor. The orientation is not stored explicitly, but is obtained when required by diagonalizing the void tensor using Equation 13. In order that the orientation not be lost as principal voids are closed, voids are not allowed to completely close once they have opened; that is, principal void strains will be greater than some limit $\varepsilon_\pi \sim 10^{-10}$. The orientation is corrected for the rigid body rotation of Equation 11.

Principal Stress Flow Rules

In this section, the flow rules are expressed in terms of the changes in the principal stresses (or at least the components of the stress tensor along the principal void tensor axes). Several types of flow rule are

considered: (A) deviator stress relaxation in which no shear stress is allowed along a fully developed crack or equivalently that the principal stress and void coordinate systems coincide, (B) tensile failure in which a stress component exceeds the tensile strength of the material, (C) void closure in which a compressive stress is found normal to an open void, (D) pure shear failure in which the shear stress between pairs of stress components is relaxed, (E) shear closure in which the closure of a void has produced a shear stress which exceeds the shear strength, and (F) closure constraints in which voids are prevented from overclosing.

First a target stress is defined, then a target stress change $\Delta\sigma$ which must be decomposed into its volumetric $\Delta\sigma^T$ and shear $\Delta\sigma^S$ components,

$$\Delta\sigma = \Delta\sigma^T + \Delta\sigma^S \quad (28)$$

corresponding to the decomposition of Equation 9. The decomposition is chosen such that $\Delta\sigma^T$ is diagonal and $\Delta\sigma^S$ has zero trace. The corresponding changes in the inelastic void π and shear strain ε^S tensors are obtained by using the elasticity matrix (Equation 7)

$$\begin{aligned} \Delta\pi &= \Lambda \mathbf{D}^{-1} \Delta\sigma^T \\ \Delta\varepsilon^S &= \Lambda \mathbf{D}^{-1} \Delta\sigma^S \end{aligned} \quad (29)$$

in which Λ is a Lagrange multiplier used to invoke a constraint which prevents closing voids which are already closed. In the following the use of Λ will be seen to be equivalent to breaking the timestep into smaller steps of $\Lambda\delta t$.

(A) Deviator Stress Relaxation. There are two factors which must be considered. Recall that if $\varepsilon^D < \varepsilon_{oT}^D$, then our coordinate system was taken to be that of the stress tensor and $\tau_{12}=0$ so that no relaxation is necessary. Secondly, if the voids are closed, the shear stress will take on its frictional value. However, this has already been taken care of by the shear failure algorithm which has just been applied. Accordingly, the flow rule (Figure 7) is given by,

DEVIATOR RELAXATION

$$(\pi_1, \pi_2 > 0 \text{ and } \varepsilon^D > \varepsilon_{oT}^D)$$

$$\Delta\tau_{12} = [\tau_{12} - Y^e(1 - \varepsilon^D/\varepsilon_{oT}^D)]\delta t/\tau$$

$$\rightarrow [\tau_{12} - 0]\delta t/\tau$$

$$\Delta\tau_{12}^T = 0$$

$$\Delta\tau_{12}^S = \Delta\tau_{12}$$

(30)

$$(\pi_i=0 \text{ or } \varepsilon^D < \varepsilon_{0T}^D)$$

$$\Delta\tau_{12} = \Delta\tau_{12}^T = \Delta\tau_{12}^S = 0$$

in which δt is the timestep and τ is a Maxwell relaxation time.

Figure 7. Deviator Stress Relaxation.

(B) Tensile Failure. In the flow rule for tensile failure (Figure 8) the stress components σ_i are compared with the effective tensile strength in that direction T_i^e . If $\sigma_i > T_i^e$, the material fails in tension. The target stress is T_i^e , and the amount of the stress relaxation is taken to be,

TENSILE FAILURE

$$(\sigma_i > T_i^e)$$

$$\Delta\sigma_i = (\sigma_i - T_i^e)\delta t/\tau > 0 \quad (31)$$

$$\Delta\sigma_i^T = \Delta\sigma_i$$

$$\Delta\sigma_i^S = 0$$

Thus, the stress σ_i is relaxed toward the effective tensile strength T_i^e .

The relaxation time allows the incorporation of rate effects in the model and reduces numerical noise which can occur if the stress state is simply "pinned" to the tensile strength (i.e., $\tau = \delta t$).

Figure 8. Tensile Failure.

(C) Void Closure. If the stress $\sigma_i < 0$ (i.e., compressive) and there are open voids $\pi_i > 0$, then there is a compressive stress on an open crack and void closure must occur. As shown in Figure 9, here the target stress is 0,

VOID CLOSURE

$$(\sigma_i < 0 \text{ and } \pi_i > 0)$$

$$\Delta \sigma_i = (\sigma_i - 0) \delta t / \tau < 0 \quad (32)$$

$$\Delta \sigma'^T_i = \Delta \sigma_i$$

$$\Delta \sigma'^S_i = 0$$

The shear failure algorithm (page 25) has already guaranteed that the differences between the stress components satisfy the yield criterion at least approximately. (The caveat is necessary because the shear failure was defined in terms of invariants rather than individual stress differences.)

The above flow rules, however, alter the stress components and therefore admit the possibility of exceeding the material shear strength. While this applies to both rules (A) and (B), the tensile rule (A) is likely

Figure 9. Void Closure.

to be a problem only under very unusual conditions; and its effects are presently ignored. The closure rule (B) requires more careful consideration. When one compressive stress is relaxed toward 0, it is quite likely that some of the other stresses are even more compressive. The stress difference is then increased and the possibility of exceeding the shear strength occurs. The solution of course is to apply the shear failure criterion to the differences of the stress components. The following shear flow rule is applied to stresses σ_j ($j \neq i$) which have not been constrained by the tensile or void closure flow rules.

(D) Pure Shear failure First define the flow rule for a pure shear relaxation by an amount $\Delta\sigma$, (Figure 10).

PURE SHEAR FAILURE

$$(j \neq 1)$$

$$\Delta\sigma_1 = \Delta\sigma$$

$$\Delta\sigma_j = -\Delta\sigma$$

(33)

$$\Delta\sigma'^T_i = \Delta\sigma'^T_j = 0$$

$$\Delta\sigma'^S_1 = \Delta\sigma$$

$$\Delta\sigma'^S_j = -\Delta\sigma$$

As indicated earlier, it seems preferable to define all shear failure in terms of stress differences rather than invariants; and this type of rule may eventually be used to describe all shear failure. While this rule is not used explicitly at present, it is used conceptually to devise the following flow rule for shear closure of voids.

Figure 10. Pure Shear Failure.

(E) Shear Closure. The desired final state is obtained by applying void closure C twice and pure shear failure D once. The net effect of this is to slide the Mohr circle so that one of the stress components is at the the origin (Figure 11). Although Y^e should be corrected for the slope of the yield surface as shown in Figure 12, this is not presently done.

SHEAR CLOSURE

$$(\Delta\sigma_i < 0, \Delta\sigma_j = 0, j \neq i, \text{ and } |(\sigma_i - \Delta\sigma_i) - \sigma_j| > 2Y^e)$$

$$\Delta\sigma_i = \sigma_i \delta t / \tau$$

$$\Delta\sigma'^T_i = 2\Delta\sigma_i$$

$$\Delta\sigma'^S_i = -\Delta\sigma_i$$

(34)

$$\Delta\sigma_j = \Delta\sigma_i$$

$$\Delta\sigma'^T_j = 0$$

$$\Delta\sigma'^S_j = \Delta\sigma_i$$

in which Y^e is the effective shear strength defined in Equation 24.

Figure 11. Shear Closure.

Figure 12. Corrected Shear Closure.

Rules C and D operate on pairs of stress components. When one of these is the intermediate stress, the stress difference between it and the third stress will be increased. This requires that the shear failure criterion be applied to all pairs of stress components.

(F) Closure Constraints. It may not in fact be possible to achieve the target stress changes because of the three constraints on void closure,

$$\Delta\pi_1 + \pi_1 \geq \varepsilon_\pi \quad (35)$$

in which ε_π ($\sim 10^{-10}$) is the minimum closure strain and is necessary to avoid losing the fracture orientation after all voids close.

Failure to observe these constraints can result in the calculation of excessively large stresses on the next cycle. The Lagrange multiplier in Equation 29 is unity unless required to satisfy the above constraints.

$$\Lambda_i = \text{Min}\{1, (\varepsilon_{\pi} - \pi_i)/D_{ij}^{-1}\Delta\sigma_j\} \quad (36)$$

If any Λ_i is zero, a special solution described later is called for. Otherwise, the smallest nonzero value controls the solution.

Then Equation 29 can be applied to provide the relaxed stress and void tensor components,

$$\begin{aligned} \pi' &= \pi + \Delta\pi \\ \sigma' &= \sigma - (\Delta\sigma^T + \Delta\sigma^S) \end{aligned} \quad (37)$$

which are the final states if no constraints were invoked. If the Λ_i constraints were involved, the result of Equation 37 is regarded as an intermediate state, and the flow rules reapplied.

Special Case $\Lambda = 0$. This situation must be handled by a different procedure. This case is not as unusual as it might seem. A virgin material failing for the first time in tension will have a solution like $\Delta\pi_1 > 0$ (tensile failure) and $\Delta\pi_2, \Delta\pi_3 < 0$ (closure). But for a virgin material, $\pi_2 = \pi_3 = 0$ and we must have $\Lambda = 0$. There are two possibilities to consider: $\Lambda_i = 0$ and $\Lambda_i, \Lambda_j = 0$. The third possibility of all three Λ being zero should not occur.

While the target stress change can still be attained, the proposed assignment to void and shear stress adjustments cannot. It is necessary to transfer the strain $\Delta\pi_i$ associated with the void strain tensor π to the shear strain tensor ε^S , without changing $\Delta\sigma$. In the case of a single zero Λ , the solution is not unique, and it is assumed that the tensile stress adjustment is to be split proportionately between the j and k components as follows,

Special Case 1

$$(\Lambda_i = 0, j, k \neq i)$$

$$\Delta\sigma_i, \Delta\sigma_j, \Delta\sigma_k \text{ unchanged}$$

$$\lambda = (1 - \lambda/3k)(\Sigma\Delta\sigma'^T)/(\Delta\sigma'^T_j + \Delta\sigma'^T_k) \quad (38)$$

$$\begin{aligned}\Delta\sigma'_i{}^T &= \lambda^2(\Delta\sigma'_j{}^T + \Delta\sigma'_k{}^T)/(3k-\lambda) \\ \Delta\sigma'_{j,k}{}^T &= \lambda \Delta\sigma'_{j,k}{}^T \\ \Delta\sigma'_{i,j,k}{}^S &= \Delta\sigma'_{i,j,k}{}^S + \Delta\sigma'_{i,j,k}{}^T - \Delta\sigma'_{i,j,k}{}^T\end{aligned}$$

With two zero Λ , the solution is unique and is given by,

Special Case 2

$$(\Lambda_i, \Lambda_j = 0, k \neq i, j)$$

(39)

$$\begin{aligned}\Delta\sigma'_k{}^T &= (3k-2\lambda)(\Sigma\Delta\sigma'{}^T)/(3k-\lambda) \\ \Delta\sigma'_{i,j}{}^T &= \lambda\Delta\sigma'_k{}^T/(3k-2\lambda) \\ \Delta\sigma'_{i,j,k}{}^S &= \Delta\sigma'_{i,j,k}{}^S + \Delta\sigma'_{i,j,k}{}^T - \Delta\sigma'_{i,j,k}{}^T\end{aligned}$$

Damage Formulation

In the case of metals whose composition can be carefully controlled, damage models can be precisely calibrated [40]. With geologic material, however, there has usually been little to work from except for qualitative estimates of inelastic strain associated with certain visual categories of fracture[78]. Aside from compression and triaxial data on "competent" and "rubblized" samples, there is almost no data on post-failure material behaviour. Recent work on calibrating statistical models shows promise, but is not yet generally applicable[...].

As presently formulated, the damage which causes the effective shear and tensile strengths to decrease is relatively arbitrary because existing experimental data for earth materials usually does not warrant a more detailed description. As better statistical models are formulated, it should be possible to replace this damage definition with more definitive physics, without significantly altering the general failure formulation in the code.

As indicated previously (Equations 24 and 31), the shear and tensile strengths are reduced depending upon amount of damage undergone. At present, the damage is carried as a scalar which is incremented during the failure calculations and which is a weighted sum of inelastic strains due to shear and tensile failure,

$$\varepsilon^D = D_1 \varepsilon_{oS}^D + D_2 \varepsilon_{oT}^D \quad (40)$$

in which the weighting coefficients for shear and tensile damage are $D_1 \sim D_2 \sim 1$. The code actually provides for separate sets of D coefficients for use in Equations 24 and 31 respectively.

The definitions of ε_{oS}^D and ε_{oT}^D are chosen so that these quantities are monotonically increasing with time; that is, so that the material cannot heal. Because voids are allowed to close as described below, it is not possible to relate damage to the current void tensor without causing fractures to heal as they close. The trace of the void tensor is

$$\pi_s = \sum \pi_i \quad (40)$$

and is termed the "fracture induced porosity." In terms of this,

$$\varepsilon_{oT}^D = \text{Max}_t \{ \pi_s(t) \} \quad (42)$$

One measure of damage due to shear failure is the plastic shear strain $J_2'(\varepsilon^P)$. As we consider the void strain explicitly, our form would involve the inelastic shear strain tensor $J_2'(\varepsilon^S)$. As these are not guaranteed to be monotonically increasing functions of time, a differential form is used,

$$\begin{aligned} \delta \varepsilon_{oS}^D &= \delta [J_2'(\varepsilon^S)]^{1/2} \\ \varepsilon_{oS}^D &= \sum_t |\delta \varepsilon_{oS}^D| \end{aligned} \quad (43)$$

No attempt has been made to incorporate damage due to pore collapse in the present formulation. Compaction if maintained could be expected to increase the shear strength but degrade the tensile strength.

Internal Energy

In multiphase problems, such as those involving pore fluids, each constituent will have its own internal energy relation expressed in terms of its own stress and strain rates. As past applications of *TENSOR* have not demanded that this distinction be made, only the internal energy of the composite material is presently carried. This internal energy equation is given by,

$$E = -P\theta + (2S_r + S_z)\dot{\epsilon}_r + (2S_z + S_r)\dot{\epsilon}_z + 2S_{rz}\dot{\epsilon}_{rz} \quad (44)$$

and is integrated to arrive at the new internal energy (per original unit volume) for each zone. All quantities in this equation are centered at $n-1/2$. As indicated earlier, the appropriate viscosities are added to each stress in Equation 44 before the integration. The need for this centering on Q was first pointed out by Trulio and Trigger^[32] who showed that the pressures and artificial viscosities should enter the energy equation in the same way as they are used in the momentum equation.

Artificial Viscosity

Historically, artificial viscosity or Q has made possible the calculation of shock phenomena using explicit difference methods. In recent years other methods have been developed such as implicit differencing (page 58) and flux-corrected transport (FCT, page 42), but Q remains the conventional way to handle such discontinuities.

VonNeumann Richtmyer Form. Before presenting the Q formulation used in *TENSOR*, some of the normal and pathological properties of Q will be discussed. Nearly all Q formulations are similar in form to that originally devised by VonNeumann and Richtmyer (VNR)^[83]. In one dimension, this Q is composed of terms which are various powers of the velocity difference between adjacent nodes. Since rarefactions do not usually give rise to numerical instability, the Q is given an asymmetric form in which the velocity difference is set to zero if the zone is expanding. There does not

appear to be a fundamental need for this asymmetry, and in fact the properties of a symmetric form are discussed later. However, in some problems, such as the calculation of spall phenomena, the asymmetric form is essential if unrealistic free-surface decelerations are to be avoided.

It is commonly recognized that the role of artificial viscosity is to yield an approximation for the time advanced stress which might be found in a fully implicit scheme. By applying the Rankine-Hugoniot conditions to the cases of shocks propagating through a gas^[92] and through a linear solid^[91] one can show that the pressure behind the shock has a form which can be written as $P+Q$ where Q is similar in form to the VNR viscosity.

In the discussion of Figure 1 it was pointed out that the time centering of P and Q are at n and $n-1/2$ respectively, an apparent violation of the intended central difference scheme. The necessity for this centering was pointed out by Noh^[94] who argued that for $P \ll Q$ the explicit difference form of the momentum equation (Equation 4) reduces to the heat equation which becomes unstable if Q is centered at n instead of $n-1/2$. This, however, is true only for explicit differencing. Chin and Hedstrom^[95,96] have devised an implicit form using a hopscotch method^[97] in which Q for alternate zones is centered at n and $n-1/2$ on alternate cycles. This form is not presently used in *TENSOR* but should be given consideration in the future. [Instead of a VNR variation, Chin and Hedstrom used a Laplacian formulation which also has diffusive properties.]

Zone Size Dependence. The VNR form can be rewritten in a Navier-Stokes form (in terms of strain rates) simply by expressing the velocity difference Δu as the product of a principal strain rate $\dot{\epsilon}$ times the zone size Δx ,

$$\Delta u \rightarrow \dot{\epsilon} \Delta x \quad (45)$$

As evident from Equation 45, the VNR Q is zone size dependent. One adverse effect of this occurs in gas dynamics problems in which a considerable variation in zone size is produced by a propagating shock through an originally uniform mesh. The calculated pressures are found to be systematically biased due to the presence of the zone size in the Q formulation^[102]. This bias is seen to disappear when one goes to a viscoelastic (Voigt) form by simply replacing the zone size in Equation 45 by a characteristic length L ,^[78]

$$\Delta u \rightarrow \dot{\epsilon} L \quad (46)$$

The principal disadvantage of this procedure is that smaller zones may be

overdamped; and the timestep becomes unnecessarily reduced since the Q coefficients enter the stability criterion (Equation 50).

A second result of the zone size dependence is that the effect of Q cannot easily be studied analytically for irregular grid spacing. If the Voigt form for the linear Q is used and the asymmetric constraint is dropped, the differential equations corresponding to the difference equations can be written and analytical solutions obtained.^[93] As a practical formulation, however, the symmetric Voigt Q is probably not acceptable for many applications. While conserving impulse, the attenuation of peak shock pressures and velocities with range is much greater than with the VNR form.

Multi-Dimensional Form

In two and three dimensions the choice of a proper formulation is much less clearcut than in one dimension. Clearly a form expressed in terms of strain rates offers substantial conceptual advantages, but which representation of the strain rate tensor should be used? The optimum choice depends upon the principal modes of strain anticipated in a given problem. One form formerly used in *TENSOR* [4,71] separated the strain rate tensor into its volumetric and deviatoric components, assigning separate Q coefficients to each. As will be noted later, this form offered substantial advantages of not interfering with late time relatively incompressible flow, but did not offer the desired directional response in situations involving multiple shock waves.

Unnecessary shock heating is an undesirable side effect associated with Q . The heating occurs as a consequence of the presence of viscosity in the expression for internal energy (Equation 44). In 2-D, for example, there is no motion associated with the 3 or θ direction, so that the associated viscosity is unneeded and should be set to zero to avoid artificial heating in implosion problems. In order to introduce the directional properties into Q and to address the implosion heating problem, Richards^[99] developed a directional Q which is now used in the HEMP code^[91]. In simple terms, it amounts to calculating the velocity difference only in the direction of the zonal acceleration. This removes the heating problem, but does not address multiple shocks.

Another form which attempts to account for the directional properties of the waves is the K-L form originally used in *TENSOR*.^[3] This Q looks at the velocity differences relative to the logical mesh. While reasonable for problems in which the zoning can be selected to match the anticipated strains, the formulation is not invariant and therefore guaranteed to cause problems in more general loading situations such as those in which shocks

propagate diagonally across zones. This form violates the Cardinal Rule of Modeling: "If discontinuous behavior is admitted in the numerical algorithm, it is guaranteed to show up somewhere in the problem."

A situation analogous to shock heating occurs in modeling the late quasi-incompressible flow stages of cavity or crater growth. In this configuration, there is a substantial expansive strain rate in the tangential directions and a compressive strain rate in the radial direction. There are, however, no shocks and no need for Q ; so that the volumetric Q appears well-tailored to this situation.

The TENSOR Form. While no formulation can resolve all the aforementioned difficulties, the one presently used in *TENSOR* addresses many of them directly and provides substantial user flexibility in addressing the others. The formulation is a Navier-Stokes form in which the velocity difference is replaced by a strain rate times a characteristic length, L . Operationally, one simply diagonalizes the strain rate tensor to obtain its principal components $\dot{\epsilon}_1$, $\dot{\epsilon}_2$, and $\dot{\epsilon}_3$ (which are rotational invariants). It is only in the coordinate system of the principal strain rates that meaningful decisions as to expansion or compression can be made. Defining,

$$\Delta u_i = f(\dot{\epsilon}) \dot{\epsilon}_i L_i \quad (47)$$

in which L_i is the zone width (or optionally a characteristic length) in the i th direction, and will be defined later. For implosion problems, one could choose to use only the Δu most nearly parallel to the direction of acceleration, but this option is not presently implemented.

The function f is intended to discriminate between shock and steady-state flow situations. It reduces Q toward zero as the volumetric strain rate $\dot{\theta}$ becomes small with respect to the shear strain rate.

$$f(\dot{\epsilon}) = \frac{2}{1 + |(\dot{\epsilon}_1 - \dot{\epsilon}_2)/C_3 \dot{\theta}|} \quad (48)$$

$$\rightarrow \begin{cases} 2 & \text{pure volumetric strain} \\ 1 & \text{uniaxial (shock) strain} \\ 0 & \text{pure shear strain} \end{cases}$$

in which C_3 is an adjustable coefficient (~ 1). The rationale behind this form is quite simple: when shocks are not present, the volumetric strain rate will always be small with respect to shear strain rates.

The simplest choice for L_i is the square root of the zonal area, but this is unsatisfactory for zones with large aspect ratios. While L_i can be chosen to be some global characteristic length, the disadvantages outweigh the advantages in typical *TENSOR* problems. The best choice seems to let L_i be the zone width in the i th direction. There are many possible ways to calculate this quantity, but the following has been found to be one of the most efficient. The zone diagonals are projected along the principal strain rate directions, thus defining a box surrounding the zone. The box is then shrunk so that its area matches the area of the zone. The sides of this box are L_i . This algorithm has been found to produce acceptable results for all zone shapes and orientations.

In terms of the above quantities, the components of the Q tensor are defined to be,

$$Q_i = C_1^\pm \rho c \Delta u_i + C_2^\pm \rho \Delta u_i^2 \quad i=1,2 \quad (49)$$

$$Q_3 = 0$$

in which $C_1^\pm$ and $C_2^\pm$ are the linear and quadratic Q coefficients and can be taken to have different values depending upon the sign of Δu_i . For example, the asymmetric VNR type of Q is obtained by choosing the expansional coefficients $C_1^+ = 0.2$. Typical compressional values are $C_1^- \sim 0.2$ and $C_2^- \sim 1$. As discussed later, the stability criterion depends upon the Q coefficients, and particular care must be taken because problems will tend to become unstable as the linear Q coefficient approaches unity.

Porous Materials

[100]

Flux-Corrected Transport

Hourglass Viscosity

[101] [91] [3] [98]

Stability

Text will come later. \$ (50)

Thermal and Fluid Flow Effects

Geological materials generally consist of a soil or rock matrix containing cracks and pores which may be partially or fully saturated with fluids. In describing constitutive behavior of such systems, actions of three physical processes must be considered (mechanical, thermal, and fluid flow) as well as the specific interactions between them (thermal-mechanical, thermal-fluid, and fluid-mechanical). In some applications, it is sufficient to consider these processes independently, but many geomechanics problems warrant analyses considering the coupled behavior. Work is currently underway to develop a fully coupled thermal-mechanical-fluid flow model within the framework of the *TENSOR* code.

Scaling Techniques

Modulus

Density

SPATIAL DISCRETIZATION

[THIS SECTION INCOMPLETE]

Momentum Equation

There are a great many ways to discretize the momentum equation, some clearly better than others. Most finite difference methods start with Equation 4. A few start with this equation and simply write *ad hoc* difference expressions for the derivatives. Others[...] arrive at the difference expressions for individual derivatives by carrying out two-dimensional line integrals through zone centers and surrounding the point to be accelerated.

Formally, one can write the momentum equation as a volume integral which can be converted to a surface integral using the divergence theorem. This is the so-called *conservation form* of the difference equations. Some codes[...] recognize the derivative terms in Equation 4 to represent a two-dimensional divergence and carry out a surface integral to evaluate them. In most cases the integration path passes through nearest neighbor nodes and zone centers at which stresses are centered.

A typical finite element procedure derives from the *method of weighted residuals* and amounts to assigning weighting functions and then carrying out the surface integral about zone or element boundaries with the entire Equation 4 as the integrand. Unlike finite difference methods, the path does not usually pass through the points at which stress data is centered. Stresses are carried at an arbitrary number of Gauss points within the element.

The procedure presently used in *TENSOR* uses *ad hoc* derivatives but employs weighting functions to evaluate their effect at the point to be accelerated. With minor modification the *TENSOR* procedure could be cast in an integral form in which the integration path passes through zone and side centers. It has been shown[...] that by using a coordinate transformation

the usual integral form described above can achieve the effects of weighting in the *TENSOR* form.

While appropriate for plane-strain geometry, all of the methods starting from Equation 4 omit terms which are potentially important near the symmetry axis of axisymmetric problems. If one writes difference expressions based upon a surface integral of Equation 3 rather than 4, it is obvious that the arc length in the θ direction and therefore the surface area is a function of radius from the symmetry axis. It is this fact which is omitted when starting from Equation 4. This common omission has recently been pointed out by Hart[...]. It is planned to correct this omission in the *TENSOR* differencing in the near future.

The *TENSOR* Form.

A Lagrangian coordinate system (k, ℓ) is established in the material. These coordinates move with the material and assume discrete values at the zone faces. 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 $r_{k, \ell}^0, z_{k, \ell}^0$ where the Eulerian coordinates are referred to a fixed point. After n cycles, the Eulerian coordinates of the k, ℓ point are $r_{k, \ell}^n, z_{k, \ell}^n$.

Each stress component (Σ) 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,

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

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

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

$$\frac{\partial \Sigma}{\partial r} = \frac{1}{J} \left(\frac{\partial \Sigma}{\partial k} \frac{\partial z}{\partial \ell} - \frac{\partial \Sigma}{\partial \ell} \frac{\partial z}{\partial k} \right) \quad (51)$$

and

$$\frac{\partial \Sigma}{\partial z} = -\frac{1}{J} \left(\frac{\partial \Sigma}{\partial k} \frac{\partial r}{\partial \ell} - \frac{\partial \Sigma}{\partial \ell} \frac{\partial r}{\partial k} \right), \quad (52)$$

where the Jacobian of the transformation (J) is given by

$$J = \frac{\partial r}{\partial k} \frac{\partial z}{\partial l} - \frac{\partial r}{\partial l} \frac{\partial z}{\partial k}. \quad (53)$$

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. Time is incremented in the following way:

$$\begin{aligned} t^{n+1} &= t^n + \Delta t^{n+\frac{1}{2}} \\ t^{n+\frac{1}{2}} &= t^{n-\frac{1}{2}} + \Delta t^n, \\ \Delta t^n &= \frac{\Delta t^{n+\frac{1}{2}} + \Delta t^{n-\frac{1}{2}}}{2}, \end{aligned} \quad (54)$$

where $\Delta t^{n+\frac{1}{2}}$ is determined from the stability condition.

The indices used to indicate spatial location within the logical mesh and given in Figure 13. Variables that are defined at mesh points are r, z, Δr , Δz , u, v, $\frac{du}{dt}$, $\frac{dv}{dt}$. Therefore,

Figure 13. Nodal and zonal numbering scheme. Note that the same number can refer to either a node or a zone depending upon the context.

$$\begin{aligned}
r_9^{n+1} &= r(t^{n+1}, k-1, l+1), \\
\Delta r_9^{n+1} &= r_9^{n+1} - r_9^n, \\
a_r^n &= \frac{u_1^{n+\frac{1}{2}} - u_1^{n-\frac{1}{2}}}{\Delta t^n} = \frac{du}{dt}, \\
a_z^n &= \frac{v_1^{n+\frac{1}{2}} - v_1^{n-\frac{1}{2}}}{\Delta t^n} = \frac{dz}{dt}, \text{ etc.}
\end{aligned} \tag{55}$$

Equation (55) is the interpretation of the Lagrangian derivative of an Eulerian tensor component at a material point. 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.

$$\begin{aligned}
V_1^n &= V_{k-\frac{1}{2}}^n, \quad t_{-\frac{1}{2}} = \frac{3}{\pi} \times (\text{zone volume}), \\
M_1 &= \rho_1^n V_1^n = \frac{3}{\pi} \times (\text{zone mass}), \\
P_7^n &= P_{k+\frac{1}{2}}^n, \quad l+\frac{1}{2} \\
J_8^n &= J(t^n, k-\frac{1}{2}, l+\frac{1}{2}) \\
&= \text{zone area } (2J_8^n \text{ is carried in the code}), \text{ etc.}
\end{aligned}$$

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 Equation (55) can be used to obtain the velocity at $t^{n+\frac{1}{2}}$ 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 $(2S_r + S_z)/\rho r$ and $S_{rz}/\rho r$. These terms are not affected by the coordinate transformations (Equation 51) and (Equation 52). 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 Pappas is used to define an average radius in a zone, then

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

and

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

The interior accelerations associated with zone 7 are

$$\dot{u}_7 = \frac{6J_7}{M_7}(2S_r + S_z)_7 \quad (56)$$

$$v_7 = \frac{6J_7}{M_7}(S_{rz})_7 . \quad (57)$$

The derivative terms are obtained by operating on Equation 4 with the coordinate transformation defined by Equations (51) and (52). 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, if

$$\begin{aligned} R_{81} &= 2\left(\frac{\partial r}{\partial l}\right) \\ &= r_8 - r_1 + \frac{r_7 - r_8 + r_2 - r_2}{2} \end{aligned}$$

and

$$\begin{aligned} R_{61} &= 2\left(\frac{\partial r}{\partial k}\right) \\ &= r_6 - r_1 + \frac{r_7 - r_8 + r_5 - r_4}{2} \end{aligned}$$

along with similar definitions for Z_{81} and Z_{61} , then the below equations become

$$\dot{u}_{81} = \frac{2}{(\rho J)_7 + (\rho J)_8} \frac{\partial(P-S_r)}{\partial k} \frac{\partial z}{\partial l} + \frac{\partial S_{rz}}{\partial k} \frac{\partial r}{\partial l}$$

$$\begin{aligned}
& \frac{[(P-T_r)_7 - (P-T_r)_8]_{\bar{z}_{81}} + [(T_{rz})_7 - (T_{rz})_8]_{\bar{r}_{81}}}{M_7 J_7 / V_7 + M_8 J_8 / V_8} \\
\dot{u}_{81} &= \frac{2}{(\rho J)_7 + (\rho J)_8} \frac{\partial(P-S_r)}{\partial \ell} \frac{\partial z}{\partial k} + \frac{\partial S_{rz}}{\partial \ell} \frac{\partial r}{\partial k} \\
& \frac{[(P-T_r)_7 - (P-T_r)_8]_{\bar{z}_{81}} + [(T_{rz})_7 - (T_{rz})_8]_{\bar{r}_{81}}}{M_7 J_7 / V_7 + M_8 J_8 / V_8} \\
\dot{v}_{81} &= \frac{2}{(\rho J)_7 + (\rho J)_8} \frac{\partial(P-S_z)}{\partial k} \frac{\partial r}{\partial \ell} + \frac{\partial S_{rz}}{\partial k} \frac{\partial z}{\partial \ell} \\
& \frac{[(P-T_z)_7 - (P-T_z)_8]_{\bar{z}_{81}} + [(T_{rz})_7 - (T_{rz})_8]_{\bar{r}_{81}}}{M_7 J_7 / V_7 + M_8 J_8 / V_8} \\
\dot{v}_{81} &= \frac{2}{(\rho J)_7 + (\rho J)_8} \frac{\partial(P-S_z)}{\partial \ell} \frac{\partial r}{\partial k} + \frac{\partial S_{rz}}{\partial \ell} \frac{\partial z}{\partial k} \\
& \frac{[(P-T_z)_7 - (P-T_z)_8]_{\bar{z}_{81}} + [(T_{rz})_7 - (T_{rz})_8]_{\bar{r}_{81}}}{M_7 J_7 / V_7 + M_8 J_8 / V_8}
\end{aligned} \tag{58}$$

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

$$(\dot{u}_{81})_{k-1, \ell} = (\dot{u}_{12})_{k, \ell}$$

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

Also

$$(\dot{u}_7)_{k,l-1} = (\dot{u}_8)_{k,l}$$

$$(\dot{u}_7)_{k-1,l-1} = (\dot{u}_1)_{k,l}$$

$$(\dot{u}_7)_{k-1,l} = (\dot{u}_8)_{k,l}$$

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 [a_r , and a_z]. 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 a_r , and a_z .

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

$$E_{81} = \frac{\vec{R}_{82} \cdot \vec{R}_{81}}{\vec{R}_{82} \cdot \vec{R}_{82}} = \frac{\bar{r}_{82}\bar{r}_{81} + \bar{z}_{82}\bar{z}_{81}}{(\bar{r}_{82})^2 + (\bar{z}_{82})^2}$$

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

The weighting factor for $\dot{u}_{81}$ is $1-E_{81}$ while E_{81} is the weight of $\dot{u}_{12}$. Since the nonderivative terms are interior terms, they are weighted with E_{81} and E_{81} combinations, i.e., $(1-E_{81})(1-E_{81})$ is the weight of $\dot{u}_7$. The KL_r and KL_z are damping terms used to prevent a special type of zone deformation.

The velocity of the k,l point is calculated using Equation (55).

$$u^{n+1/2} = u^{n-1/2} + \Delta t^n a_r^n$$

$$v^{n+1/2} = v^{n-1/2} + \Delta t^n a_z^n$$

Equations (56) through (58) 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.

Strain Rates

In the code, the strain rates are calculated using time-centered zone coordinates at $t^{n+\frac{1}{2}}$ and coordinate velocities $u^{n+\frac{1}{2}}$ and $v^{n+\frac{1}{2}}$.

$$\theta = e_{rr} + e_{\phi\phi} + e_{zz} = v^{-1} \frac{dv}{dt} \quad (60)$$

$$e_r = e_{rr} - \frac{\theta}{3} = \frac{1}{3} \left(2 \frac{\partial u}{\partial r} - \frac{\partial v}{\partial z} - \frac{u}{r} \right) \quad (61)$$

$$e_\phi = e_{\phi\phi} - \frac{\theta}{3} = - (e_r + e_z) \quad (62)$$

$$e_z = e_{zz} - \frac{\theta}{3} = - \frac{1}{3} \left(2 \frac{\partial v}{\partial z} - \frac{\partial u}{\partial r} - \frac{u}{r} \right) \quad (63)$$

$$e_{rz} = \frac{1}{2} \left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r} \right) \quad (64)$$

Using $(ud)_1^n$ and $(vd)_1^n$ from above, zone velocities and coordinates are calculated as follows:

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

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

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

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

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

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

In the remainder of this section, if the superscript is omitted it is understood to be $n+\frac{1}{2}$. 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 Figure 3a, the zone volume is calculated explicitly at cycle zero (the beginning of the problem) as

$$V_7^0 = r_{781}^0 \begin{vmatrix} r_{78}^0 & r_{71}^0 \\ z_{78}^0 & z_{71}^0 \end{vmatrix} + r_{761}^0 \begin{vmatrix} r_{71}^0 & r_{76}^0 \\ z_{71}^0 & z_{76}^0 \end{vmatrix} = \frac{2}{\pi} \times (\text{zone volume})$$

If

$$\Delta V_7 = V_7^{n+1} - V_7^n. \quad (65)$$

Then substituting

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

into Equation (65) gives

$$\begin{aligned} \Delta V_7^{n+\frac{1}{2}} &= \Delta t \left\{ u_{781} \begin{vmatrix} r_{78}^0 & r_{71}^0 \\ z_{78}^0 & z_{71}^0 \end{vmatrix} + u_{716} \begin{vmatrix} r_{71}^0 & r_{76}^0 \\ z_{71}^0 & z_{76}^0 \end{vmatrix} + r_{781} \begin{vmatrix} u_{78}^0 & u_{71}^0 \\ z_{78}^0 & z_{71}^0 \end{vmatrix} \right. \\ &\quad + r_{716} \begin{vmatrix} u_{71}^0 & u_{76}^0 \\ z_{71}^0 & z_{76}^0 \end{vmatrix} + r_{781} \begin{vmatrix} r_{78}^0 & r_{71}^0 \\ z_{78}^0 & z_{71}^0 \end{vmatrix} + r_{716} \begin{vmatrix} r_{71}^0 & r_{76}^0 \\ z_{71}^0 & z_{76}^0 \end{vmatrix} \\ &\quad \left. + \left(\frac{\Delta t}{2}\right)^2 \left[u_{781} \begin{vmatrix} u_{78}^0 & u_{71}^0 \\ z_{78}^0 & z_{71}^0 \end{vmatrix} + u_{761} \begin{vmatrix} u_{71}^0 & u_{76}^0 \\ z_{71}^0 & z_{76}^0 \end{vmatrix} \right] \right\} \quad (66) \end{aligned}$$

Then,

$$DV_7^{n+1} = DV_7^n + \Delta V_7^{n+\frac{1}{2}}$$

$$V_7^{n+1} = V_7^o + DV_7^{n+1}$$

$$V_7^{n+\frac{1}{2}} = V_7^{n+1} - \frac{\Delta V_7^{n+\frac{1}{2}}}{2}, \quad (67)$$

$$MU_7^{n+1} = - \frac{DV_7^{n+1}}{V_7^{n+1}} \quad (68)$$

$$\eta_7^{n+1} = \frac{V_7^o}{V_7^{n+1}} \quad (69)$$

$$EDV_7 = \frac{\Delta V_7^{n+\frac{1}{2}}}{V_7^o}. \quad (70)$$

Equation (68) is defined to be the total volumetric strain associated with zone 8167. Notice that the code has not used Equation (60) to calculate volume changes. Equation (68) is exact in that it represents no assumption concerning the differenced form of the partial derivatives.

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

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

The deviatoric strain rates $[e_r, e_z, e_{rz}]$ in Equation (59) can be transformed into the Lagrangian coordinate system using Equations (51) and (52).

$$\begin{aligned} \frac{\partial u}{\partial r} &= \frac{1}{4J^{n+\frac{1}{2}}} [(u_{71} - u_{86})(z_{71} + z_{86}) - (u_{71} + u_{86})(z_{71} - z_{86})] \\ &= \frac{1}{2J^{n+\frac{1}{2}}} \begin{vmatrix} u_{71} & u_{86} \\ z_{71} & z_{86} \end{vmatrix}, \end{aligned} \quad (72)$$

$$\frac{\partial u}{\partial z} = \frac{1}{2J^{n+\frac{1}{2}}} \begin{vmatrix} u_{86} & u_{71} \\ r_{86} & r_{71} \end{vmatrix}, \quad (73)$$

$$\frac{\partial v}{\partial r} = \frac{1}{2J^{n+\frac{1}{2}}} \begin{vmatrix} v_{71} & v_{88} \\ z_{71} & z_{88} \end{vmatrix} , \quad (74)$$

$$\frac{\partial v}{\partial z} = \frac{1}{2J^{n+\frac{1}{2}}} \begin{vmatrix} v_{88} & v_{71} \\ r_{88} & r_{71} \end{vmatrix} , \quad (75)$$

$$\frac{u}{r} = \frac{u_8 + u_1 + u_6 + u_7}{r_8 + r_1 + r_6 + r_7} . \quad (76)$$

Hourglass Viscosity

The QKL_r and QKL_z damping terms in Equations (3-16) and (3-17) are designed to prevent the type of zone deformation shown in Figure 8. Since that 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 Figure 8, we see that the k lines 61 and 78 have opposite rotations as do the l lines 76 and 81. The QKL damping terms are designed to prevent the constant strain rotations of the k and l lines.

BOUNDARY CONDITIONS

Stress Constraints

Velocity and Position Constraints

Roller Constraints

Slip Lines

Wave Transmission

IMPLICIT TIME INTEGRATION

Earth motion problems are typically characterized by one or more of the following regimes of behavior: (1) early-time shock wave propagation, (2) later relatively incompressible steady-state flow, and (3) final establishment of equilibrium. For example, in a typical containment calculation^[1], the calculation time is about equally divided between the first two phases. Cratering calculations, however, much more heavily weight the second^[2].

Traditionally, the first regime has been modeled using explicit finite-difference codes such as *TENSOR* [3, 4, 5, 6], while the third regime is normally modeled with a direct-method finite element code. For lack of better calculational tools, the intermediate regime has tended to be also modeled with codes such as *TENSOR*. The motivation in developing an implicit differencing algorithm for the *TENSOR* code has been to provide a tool more suited to this intermediate regime.

As will be explained in more detail shortly, the implicit method offers many attractive advantages over the explicit method. Potentially, it is more accurate because one can directly control the solution accuracy. It can be faster and therefore cheaper because the calculational timesteps need not be limited by the Courant-Friedrichs-Lewy (CFL) condition [7, 8]. This is especially important in problems requiring fine zoning to define geometrical configurations and in problems in which turbulence causes pathological zone distortion and accompanying reduction in timestep. While explicit methods require artificial viscosities to smooth shock fronts into smooth waves, no such viscosity need be introduced with the implicit method. The constitutive relations for earth materials are highly nonlinear, and often require an additional timestep control which is usually ignored in practice. Such nonlinearities are handled naturally with the implicit method.

The distinction between explicit and implicit differencing methods is illustrated in Figure 14. In both cases one has a difference equation for momentum which relates acceleration at a given timestep to stress at that same time. In the explicit case, the acceleration at n is used to advance velocity from $n-1/2$ to $n+1/2$, which is in turn used to advance displacements from n to $n+1$. It turns out that it is the extrapolation of velocity and displacement information beyond the time at which there is stress and acceleration information which gives rise to the stability restriction on the timestep. However, in the implicit case there is not only stress and

acceleration at n but also the same information at $n+1$. A mixture of n and $n+1$ accelerations is used to advance velocity and similarly displacement. For the proper mixture, the implicit method is unconditionally stable for arbitrarily large timesteps. Thus, the explicit timestep is limited by the zone size and by the soundspeed with no direct control on the accuracy of the solution. The implicit timestep, however, is limited only by the desired accuracy, the desired frequency response, and by whatever additional constraints may be required to solve the system of equations.

Figure 14. Explicit-Implicit Comparison

Solution Technique

In the explicit case, there is a single algebraic equation for each acceleration component at each node (See Figure 14). The equations are not coupled between nodes and can be solved directly with relatively simple coding. With the implicit method, however, the stress is also a function of

the acceleration at that time, giving rise to an expression with acceleration on both sides of the equation, and requiring an implicit solution. Further, the equations are coupled between nodes. The solution techniques are considerably more difficult than those for the explicit method. The alternatives are either an so-called direct method such as Gauss elimination or an iterative method such as that utilized here. When nonlinear constitutive relations are involved, iteration is necessary even with direct methods.

Computational cost for the general class of problems to be solved is a principal consideration in choosing a solution method for the implicit equations. The standard for comparison will be taken to be the CPU (Central Processor Unit) time per cycle for the explicit method which is proportional to the number of nodes N . The CPU time per cycle for the direct solution to the implicit equations is proportional to N^2 for a linear constitutive relation and higher for nonlinear relations. Consider a typical case of $N=250$ ^[9] for which the CPU time per cycle was 75 times that of the explicit CPU time. This means that in order to break even with respect to cost, it is necessary to use an implicit timestep which is at least 75 times that allowed by the explicit CFL condition. This may impose an unacceptable limitation upon the obtainable frequency response.

For the above reason, an iterative method has been selected for use in *TENSOR*. The CPU time is proportional to N as in the explicit method. The proportionality constant and consequently the cost effectiveness of the method varies with a number of factors: the details of the iteration scheme, the convergence (accuracy) criteria, the linearity of the constitutive relations, the presence of discontinuities such as shocks, and the timestep in relation to the CFL timestep. The desired operating range of the code is in the realm of 1 to 10 times the CFL timestep at a CPU cost of 1 to 5 times that of the explicit method.

In advancing velocity from n to $n+1$, a number of expressions have been used successfully. One of the best is the Newmark trapezoidal rule^[10,11]

$$\begin{aligned} u_k^{n+1} &= u_k^n + [a_k^n(1-\delta) + a_k^{n+1}\delta] \delta t \\ r_k^{n+1} &= r_k^n + u_k^n \delta t + [a_k^n(\frac{1}{2}-\alpha) + a_k^{n+1}\alpha] \delta t^2 \end{aligned} \quad (77)$$

For the choice $\alpha=1/4$ and $\delta=1/2$, the method is called the "constant average acceleration" method (CAA) and is unconditionally stable for all timesteps^[12]. In order to remain compatible with the explicit differencing in *TENSOR*, it is desirable to center velocities at the half timestep. The Newmark expression can be expressed equivalently as

$$\begin{aligned}
u_k^{n+1/2} &= u_k^{n-1/2} + [a_k^n(1-\gamma) + a_k^{n+1}\gamma]\delta t \\
&\rightarrow u_k^{n-1/2} + [3a_k^n + a_k^{n+1}]\delta t/4 & \gamma \rightarrow 1/4 \\
r_k^{n+1} &= r_k^n + u_k^{n+1/2}\delta t
\end{aligned} \tag{78}$$

The choice $\gamma=1/4$ corresponds to the constant average acceleration method. In order to simplify notation, we will drop the superscript $n+1/2$, so that

$$\begin{aligned}
u_k^{n+1/2} &\rightarrow u_k \\
\{u^{n+1/2}\} &\rightarrow \{u\}
\end{aligned}$$

the latter denoting the set of all velocities in the mesh.

Suppose that the difference expression for a given nodal acceleration can be written

$$a_k^{n+1} = f_k\{\sigma^{n+1}\} \tag{79}$$

in which $\{\sigma\}$ indicates a set of all stresses in the difference grid. In *TENSOR*, each interior node is surrounded by four zones each of which contains a stress. The spatial difference expressions are first-order so that at a given node the set $\{\sigma\}$ reduces to just the adjacent four stresses. The stresses, however, are functions of the strain rates at $n+1/2$ and therefore the velocities at $n+1/2$.

$$\sigma_k^{n+1} = g_k\{u\} \tag{80}$$

Each zone is delimited by four nodes, each of which has a velocity so that for a given zone $\{u\}$ reduces to the surrounding four velocities. Then,

$$\begin{aligned}
 a_k^{n+1} &= f_k \{ g\{u\} \} \\
 &= h_k \{u\}
 \end{aligned}
 \tag{81}$$

Consequently, at a given node, the set $\{u\}$ reduces to nine velocities, that of the node itself and of the surrounding eight nearest neighbors. The implicit nature of this expression becomes apparent by making use of the Newmark rule,

$$u_k = u_k^{n-\frac{1}{2}} + [3a_k^n + h_k\{u\}]\delta t/4 \tag{82}$$

in which u_k appears on the left and on the right as one of the set $\{u\}$. In relating this expression to the equation appearing in Figure 14, one need only realize that solution for a_k^{n+1} and its integral u_k are equivalent.

Equation 82 is the set of coupled implicit equations which must be solved either by a direct method or by iteration. The iterative solution to the equations is accomplished by a form of functional iteration^[13]. At each node k , define

$$\begin{aligned}
 G_k\{u\} &= u_k^{n-\frac{1}{2}} + [3a_k^n + h\{u\}]\delta t/4 \\
 F_k\{u\} &= u_k - G_k\{u\}
 \end{aligned}
 \tag{83}$$

The problem can now be restated. It is necessary to find the roots of the set of equations

$$F_k\{u\} = 0$$

Denoting u_k^i as the i th iterate of u_k , then functional iteration will yield a convergent solution of the following form for certain matrices A .

$$u_k^{i+1} = u_k^i - A_{kj} F_j \{u\} \quad (84)$$

in which repeated indices are summed. In particular, if A is the inverse of the Jacobian, the procedure is known as a Newton or Newton-Raphson method,

$$\begin{aligned} A &= J^{-1} \\ &= \{J_{kj}\}^{-1} \end{aligned}$$

where

$$J_{kj} = \partial F_k / \partial u_j$$

If the Jacobian is not evaluated every iteration, but is kept constant for several iterations, the procedure is a quasi-Newton method, although in some literature it is also called a Newton-Raphson method^[14]. These methods have the disadvantage that the inverse of an $N \times N$ matrix must be found each iteration or after several iterations.

The method currently used in *TENSOR* derives from an acceleration procedure for non-linear systems discussed by Isaacson and Keller^[13, p.120] which amounts to using only the diagonal elements of the Jacobian.

$$\begin{aligned} A &= \{\beta \delta_{kj} J_{kk}\}^{-1} \\ &= \{\beta \delta_{kj} (1 - G_{kk})\}^{-1} \\ &= \{\beta \delta_{kj} / (1 - G_{kk})\} \end{aligned} \quad (85)$$

in which

$$\begin{aligned} G_{kj} &= \partial G_k / \partial u_j \\ &= \partial h_k / \partial u_j \Delta t / 4 \end{aligned}$$

and β is an underrelaxation factor (typically 1/2) which can be adjusted to accelerate convergence. Underrelaxation is necessary because the use of only a partial Jacobian causes each iterative correction to overshoot. If convergence is rapid enough, this method offers substantial advantages over the full Newton method, because the inverse does not need to be found numerically. In some literature^[15] this method has also been referred to as a Newton-Raphson method if the Jacobian is not evaluated each iteration. The ICE (implicit continuous Eulerian) method^[16,18,17] uses this basic procedure; however, since only fluids without shear stresses were involved, ICE iterates on the scalar pressure rather than the vector velocity.

Because of the relatively strong coupling between the horizontal and vertical velocity components u and v introduced by the presence of the full stress tensor, the method adopted here is a modification of the above in which only terms in the Jacobian which couple the two velocity components at each point are retained. The inverse is simply obtained by solving a system of just two equations at each node.

$$\begin{aligned} u_k^{i+1} &= u_k^i + \beta[(G_{uu}-1)u_k^i + G_{uv}v_k^i] \\ v_k^{i+1} &= v_k^i + \beta[G_{vu}u_k^i + (G_{vv}-1)v_k^i] \end{aligned} \quad (86)$$

Because of the nonlinear nature of the constitutive relations, the derivatives are evaluated each iteration.

Once the $i+1$ velocities are found, the iterated stresses in zone j are determined from,

$$\begin{aligned} \Delta\sigma_j^{i+1} &= g_j\{u^{i+1}\} - \sigma_j^i \\ \sigma_j^{i+1} &= \sigma_j^i + \omega \Delta\sigma_j^{i+1} \end{aligned} \quad (87)$$

where ω is an overrelaxation factor which is used to accelerate convergence and is typically 1.5. While the stresses are updated during the iteration, history dependent equation of state variables are not permanently updated until the iteration has converged.

To this point the procedure described is similar to the Gauss-Jacobi method^[13]. To further accelerate convergence, as a new velocity is

calculated at each point, the effect on the adjacent stresses is calculated and they are immediately updated,

$$\begin{aligned}
 \Delta u_k^{i+1} &= u_k^{i+1} - u_k^i \\
 \Delta \tilde{\sigma}_j^{i+1} &= \Delta u_k^{i+1} \partial g_j / \partial u_k \\
 \sigma_j^{i+1} &\rightarrow \sigma_j^{i+1} + \omega \Delta \tilde{\sigma}_j^{i+1}
 \end{aligned} \tag{88}$$

so that the new velocity information is propagated immediately to adjacent nodes which have not yet been calculated. This is known as the point successive substitution method or as the Gauss-Seidel method^[13], a procedure which doubles the rate of convergence with respect to Gauss-Jacobi. Collectively, the procedures outlined in Equations 87 and 88 are known as successive overrelaxation (SOR). The procedure of using underrelaxation on the solution variable u and overrelaxation on the coupling variables σ is the converse of a method used by Winslow^[19] in solving elliptic equations.

During each cycle, the iteration is continued until both global and local convergence criteria are satisfied or until a maximum number of iterations is reached in which case the user has the option of continuing or not. The global criterion

$$\Sigma \delta u_k^2 / \Sigma u_k^2 < \beta \epsilon_c \quad (\epsilon_c \sim 10^{-6}) \tag{89}$$

is necessitated by the nonlinear nature of the equations and would be required even if a direct method of solution were used. The inclusion of the underrelaxation factor β is necessary because one could in principle force a false convergence by an arbitrarily small choice of β . The local criterion is necessitated only by the iterative solution method and is given by

$$\begin{aligned}
 \Delta P_j^{i+1} / P_c &< \beta \epsilon_p \quad (\epsilon_p \sim 10^{-4}) \\
 \Delta \mu_j^{i+1} / \mu_c &< \beta \epsilon_m \quad (\epsilon_m \sim 10^{-4})
 \end{aligned} \tag{89}$$

in which ΔP is the pressure change corresponding to $\Delta\sigma$, and $\Delta\mu$ is the corresponding excess compression ($\mu = \rho/\rho_0 - 1$). The quantities P_c and μ_c represent a characteristic pressure and compression, and are usually taken to be the maximum values of these quantities present in the problem.

Figure 15. Implicit Calculational Procedure

Figure 15 shows the order in which the various quantities are calculated. The previous cycle exited the iteration immediately after calculating the final (n) values for the nodal variables (a_r , a_z , u , v , r , and z) but before the final values for zonal variables are calculated (σ , E , and Q). The reason for this staggered procedure is to minimize the number of variables which must be stored from one cycle to the next. The next (n+1) cycle then begins with the calculation of the final values for stress and acceleration at n. The trial values for acceleration, velocity, coordinates, strain rates, stresses, and energies at n+1 are then determined in that order.

The calculational procedure is very similar to that used in the explicit calculation. This was done intentionally so that the same code could operate in either explicit or implicit modes by simply setting a flag. Further, since zones may vary widely in their CFL stability limits, it is practical to let some regions of a given problem follow the explicit algorithm while others are iterated upon implicitly. To reduce calculation time, each zone and node carries an activity flag which is used to avoid unnecessary iterations when it is either explicitly stable or has satisfied a local convergence criterion and has no active neighbors.

Implicit Examples

To demonstrate the applicability of the implicit *TENSOR* algorithm, five examples are given. The first three have known numerical or analytical solutions and demonstrate the accuracy of the method. The remaining two examples demonstrate possible applications of the method.

- Blake Shock Problem. An exponentially decaying pressure is applied to a spherical cavity within an infinite elastic solid.
- Broken Dam. Flow of an incompressible fluid when a vertically constraining wall is instantaneously removed.
- Impacting Rod. A cylindrical copper rod impacts a rigid boundary.
- Prototype Containment Problem. A pie slice is taken from the vertical Baneberry geology.
- Prototype Cavity Collapse. The collapse of an explosively generated cavity is calculated.

Blake Shock Problem

In the Blake problem, an exponentially decaying pressure was applied to a spherical cavity within an infinite elastic solid. Figures 16a and 16b compare the explicit, implicit, and analytical^[27, 3] solutions at 2 ms. The explicit calculation was run with the minimum Q required to suppress

serious oscillations. The implicit, however, was run with no artificial viscosity at all.

The implicit method appears to handle shocks more accurately than the explicit. The better peak of the implicit calculation is almost certainly related to the lack of Q . Unexpectedly, we have found that the peak can be further improved at the cost of some overshoot by relaxing the convergence criterion. The cost of the implicit calculation was about 3 times that of the explicit.

Both explicit and implicit timesteps were constrained at the CFL limit. Figure 16c shows a second implicit calculation run at twice the CFL timestep. Another calculation at 4 times the CFL limit (not shown) failed to converge well and produced oscillatory behavior on the trailing edge of the waveform. Our tentative conclusion is that when shocks are present the iterative implicit method is still somewhat limited by the CFL criterion.

Broken Dam

This example illustrates a completely different flow regime than that of the Blake problem. In this problem, fluid flows incompressibly under gravity after a vertical constraining wall is removed. The calculation was done both implicitly and explicitly. Figures 17a and 17b show the initial configuration and the implicit configuration at 600ms.

The implicit timestep was allowed to grow to 7 times the CFL limit. The implicit calculation ran in 6.42 minutes (CDC-7600 CPU) and 494 cycles, and cost about 1.4 times the explicit calculation. The problem has also been calculated on the SOLA-VOF Eulerian code^[29] in which nearly identical results were obtained at essentially the same CPU cost.

Figure 18 plots the scaled radial position of the leading edge versus the scaled time. Shown are experimental points^[28], implicit, and explicit results. As in the Blake problem, the implicit result is more accurate than the explicit. However, this is not always the case as is shown by a second implicit calculation in which the convergence criterion has been relaxed by a factor of 10.

Impacting Rod

This example displays both shocks and incompressible flow. A copper rod with a work-hardening constitutive relation impacts a rigid boundary. Such configurations have been used to characterize the strength properties of materials^[30]. The initial dimensions were 3.24 cm length by 0.32 cm diameter and the initial velocity was 0.227 m/ms. The problem was run to a time of 80 μ s at a timestep of 12 times the CFL limit. The configuration at this time is shown in Figure 19. The problem ran in 8.08 minutes (CDC-7600 CPU time) in 811 cycles. The implicit cost in this case was about 0.7 of what a comparable explicit *TENSOR* calculation would have been.

Comparable calculations have been previously made on the explicit DYNA finite element code^[31] in 14.0 minutes and 13000 cycles and also on the implicit (direct method) NIKE finite element code^[9] in 6.5 minutes and 80 cycles. Because of slight differences in the work-hardening formulations between *TENSOR* and the finite element codes the comparison is only approximate. The *TENSOR* work hardening parameters were selected to achieve the same final configuration as in the NIKE and DYNA calculations and therefore to simulate basically the same timestep behavior.

Prototype Containment Problem

This calculation is intended to illustrate the possible practical application of the implicit method. A pie slice is taken from the vertical Baneberry geology^[1] which contained four principal layers beginning from the surface: porous alluvium, saturated alluvium, tuff, and clay-filled tuff. The source was a gas profile selected to simulate the behavior of the Baneberry source. As the Blake shock problem suggested the early phases of the calculation could be most efficiently carried out explicitly, this was done to a time of 700ms. It was then run both explicitly and implicitly from 700ms to 1000ms. The implicit calculation was done at about 5 times the CFL limit but the CPU cost (4.4 minutes) was the same.

The cavity radius which is a critical parameter in containment analysis was nearly identical between the two calculations (33.22m and 33.20m respectively). Figures 20a and 20b show the excess compression μ plotted versus range for the two cases. The two are nearly identical. The negative μ values represent spall separation. Figures 21a and 21b show a comparison of pressure which is somewhat more sensitive than μ . While slight differences can be seen, the behavior is essentially the same.

Prototype Cavity Collapse

The collapse of an explosively generated cavity is to be calculated. The intention is not to advocate any particular collapse mechanism but rather to illustrate a potential application. Figure 22 shows the final configuration of a typical containment calculation. The problem had been run to a time of 2.64 seconds explicitly at which time the grid was essentially in equilibrium. The problem was then dezoned to produce substantially larger zones than were originally used.

As indicated, the problem is in equilibrium. No collapse can occur without further perturbation. As a first step, the cavity pressure was gradually reduced to zero over a few hundred milliseconds without significant effect. Another mechanism had to be invoked if collapse was to be observed. One choice would have been a creep mechanism in which the shear strength within a given region was gradually reduced. A second choice-- and the one arbitrarily chosen here-- was to suggest that within the heavily damaged region the material density slowly increased to its grain density. The reasoning behind such a mechanism might be the gradual flow of pore water out of the cracked material matrix. The model actually employed allowed the initial density ρ_0 to increase with time constant 100ms from 2.13 g/cc to as much as 2.85 g/cc. The final density attained depended upon the amount of damage ϵ^D , the maximum density corresponding to damage of 1 percent. This damage level was exceeded during the shock and cavity growth phases out to a range of about 150m

Figures 23 through 25 show the grid and the flow field at times of 1.6, 3.3, and 4.7 seconds after the end of the dynamic calculation (i.e., the final time was actually 4.7+2.6 seconds). A stable arch is seen to form in the material 150m above the cavity in which the damage level was less than 1 percent. The distended zones above the cavity indicate tensile failure. The highly damaged material is seen to flow downward along the side of the cavity and upward from the bottom

Concluding Remarks on the Implicit Method

As has been seen from the preceding examples, the implicit method is capable of greater accuracy or greater economy than the explicit method, but not necessarily concurrently. While a number of techniques for accelerating the convergence of the implicit iterations have been used, convergence is

not yet rapid enough to conclude that the method is consistently superior to the explicit method.

The problem in accelerating convergence is that the effect of a perturbation propagates outward at a rate of somewhat faster than one node per iteration. A way must be found to significantly increase this "radius of influence." A number of solution techniques offer potential but all require greater restructuring of the code than had been desirable until feasibility had been demonstrated. Now that this has been done, such procedures will be considered. Potential methods include block alternating direction implicit (BADI)[^{20,21}], block SOR (BSOR)[^{22,23}], and incomplete Cholesky conjugate gradient (ICCG)[^{24,25,26}] techniques.

[The following figures are available separately from the authors.]

Figure 16. Comparison of speed profiles at 2ms for the Blake problem: (a) analytical and explicit solutions, (b) analytical and implicit ($\delta t = CFL$) solutions, (c) analytical and implicit ($\delta = 2$ CFL) solutions.

Figure 17. Mesh configuration for the broken dam problem at (a) $t \sim 0$, and (b) $t \sim 600$ ms.

Figure 18. Scaled position versus scaled time for: (a) experimental data, (b) implicit solution, (c) explicit solution, (d) implicit solution with weaker convergence criterion.

Figure 19. Mesh configuration at $80\mu s$ for an impacting copper rod.

Figure 20. Excess compression ($\mu = \rho/\rho_0 - 1$) versus position at $t = 1000$ ms for a Baneberry prototype calculation: (a) explicit result, (b) implicit result.

Figure 21. Pressure versus position at $t = 1000$ ms for a Baneberry prototype calculation: (a) explicit result, (b) implicit result.

Figure 22. Typical mesh at end of a containment calculation after substantial dezoning: $t \sim 2.6$ seconds.

Figure 23. Implicit cavity collapse calculation at time $t \sim 2.6 + 1.6$ seconds: (a) portion of mesh showing cavity and region of tensile failure, (b) overlaid velocity vectors and speed contours. Approximately horizontal lines are material interfaces which were smooth before dezoning.

Figure 24. Cavity collapse at $t \sim 2.6 + 3.3$ seconds.

Figure 25. Cavity collapse at $t \sim 2.6 + 4.7$ seconds.

ARBITRARY LAGRANGIAN-EULERIAN (ALE) REZONING

Some Lagrangian hydrocodes such as *TENSOR*, employ a continuous rezoning feature which allows the code to perform in an Eulerian fashion in regions of extreme distortion. The technique involves a Lagrangian step followed by a mesh relaxation and a rezone which usually conserves mass, momentum and energy and which either averages or uses a Taylor series expansion for field quantities such as stress. The technique was originally advocated by Hirt, Amsden, and Cook^[17] and has since been employed in a number of hydrocodes^[15,84,85,86,87, 88,18] besides *TENSOR*.

Currently, mixed cells are not allowed in *TENSOR*. This places severe constraints on the remapping algorithm. Material boundaries must then match zone boundaries. The relaxation algorithm allows nodes on material boundaries to move "tangent" to them in the sense that zone areas (or volumes) are preserved on both sides of the material interface. Eventually it is hoped to introduce an algorithm which allows zones to completely "jump across" material interfaces.^[90]

The potential consequence of ALE on spall modeling comes from the choice of momentum conservation algorithm. If a given node is moved, mass and momentum will be advected between cells, requiring velocity corrections. With a second order algorithm, corrections are made at the node and at the surrounding 8 nodes. With a first order algorithm, the entire correction is made at the relaxed node only. When a problem boundary is undergoing spall, the boundary moves away from the rest of the calculational mesh. The adjacent nodes will relax so as to keep up with the boundary, resulting in a systematic momentum and mass transfer out of the outer row of cells. A second-order algorithm will adjust the boundary node velocity, thus accelerating it relative to what would have been a constant -g body acceleration. The first order algorithm does not suffer from this problem.

Mesh Relaxation

Conservation Relations

Field Variable Advection

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