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# AN EULERIAN METHOD FOR CALCULATING STRENGTH DEPENDENT DEFORMATION

## PART TWO

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## PART TWO

## DESCRIPTION OF THE FINITE DIFFERENCE EQUATIONS

by

J. M. Walsh, M. W. Evans, and J. K. Dienes

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# 1. INTRODUCTION

In the past four years several authors(1,2,3) have reported Eulerian hydrodynamic codes for the computation of compressible fluid flows in which the independent variables are two space dimensions and time.

The present paper describes the generalization of such a code(2) to include also the forces due to strength which arise within the material to resist shear deformation. In choosing the precise model for such a generalization, it is useful to recall that Eulerian codes have proven to be especially suited to the description of flows in which material elements undergo extreme distortion. It is in precisely this area of treating extreme distortions that Lagrangian codes, despite their success in treating other aspects of strength-dependent deformation,(4,5) encounter serious difficulties. In order, then, to fill the apparent need for a strength code which is capable of the simple and efficient computation of flows involving large deformations, the present code development was initiated in 1965. An informal status report was given,(6) and the code has subsequently been the subject of continuing development during the course of a number of applications.

A basic approximation underlying the present method can be mentioned here. Since the method is expected to have its primary utility in the treatment of material undergoing large deformations, it is appropriate to neglect the small elastic shear strains that may precede the onset of plastic deformation. More precisely, for a given increment in the total strain, the deviator part of the strain is assumed to be purely plastic; the remaining dilatational strain is fully accounted for in the hydrostatic equation of state. This neglect of elastic shear strains corresponds to a so-called rigid-plastic or Levy-von Mises model of the continuum, to be discussed as Section V. The present approximation does not preclude accounting for the dependence of the material strength upon the thermodynamic state of the material or upon the work done against the strength forces (work hardening). These effects are also discussed in Section 5.

A motivation in the present effort was the desire to compute the large deformations and the eventual crater size occurring in the hypervelocity impact, and the results of such a calculation are given as Ref. 14.

For completeness, both the hydrodynamic and strength aspects of the code are given in the present report, although the hydrodynamic part is largely a description of the code which was reported earlier.(2)

## 2. BASIC EQUATIONS

In an Eulerian code space is divided into fixed cells through which the fluid moves. To arrive at expressions for the rate of change of total mass, momentum and energy within such a cell, we start with the equations of motion in the form

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x_i} (\rho u_i) \tag{1}$$

$$\rho \frac{Du_j}{Dt} = \frac{\partial}{\partial x_i} (\sigma_{ij}) \tag{2}$$

$$\rho \frac{DE}{Dt} = \frac{\partial}{\partial x_i} (\sigma_{ij}\, u_j) \tag{3}$$

Here $\sigma_{ij}$ is the stress tensor, which can be regarded as the sum of the hydrostatic stress $-\ \delta_{ij}P$ and a stress deviator tensor $s_{ij}$, i.e.,

$$\sigma_{ij} = s_{ij} - \delta_{ij}P \tag{4}$$

and $E$ is the total energy per gram, kinetic plus internal. Tensor notation is implied, so that repeated indices denote summations.

In subsequent sections relations will be given for determining $P$ from the equation of state of the material and $s_{ij}$ from the material constitutive relation.

Expanding the convective derivatives in Eqs. 2 - 3, $Df/Dt = \partial f/\partial t + u_i\, \partial f/\partial x_i$, then adding Eq. 1 times $u_j$ to Eq. 2, and Eq. 1 times $E$ to Eq. 3, and collecting terms, gives

$$\frac{\partial}{\partial t} (\rho u_j) = \frac{\partial}{\partial x_i} \sigma_{ij} - \frac{\partial}{\partial x_i} (\rho u_i\, u_j) \tag{2'}$$

$$\frac{\partial}{\partial t} (\rho E) = \frac{\partial}{\partial x_i}(\sigma_{ij}\, u_j) - \frac{\partial}{\partial x_i} (\rho u_i E) \tag{3'}$$

For the developments to follow it is desirable to replace these differential equations by related integral equations, obtained by integrating over the cell volume τ, and then converting the volume integral of divergences to surface integrals over the cell surfaces. Equations 1, 2', and 3" then become

$$\frac{\partial}{\partial t}\int_\tau \rho d\tau = -\int_s \rho u_i n_i ds \qquad (5)$$

$$\frac{\partial}{\partial t}\int_\tau \rho u_j d_\tau = \int_s \sigma_{ij} n_i ds - \int_s \rho u_i u_j n_i ds \qquad (6)$$

$$\frac{\partial}{\partial t}\int_\tau \rho E d\tau = \int_s \sigma_{ij} u_j n_i ds - \int_s \rho u_i E n_i ds \qquad (7)$$

# 3. COMPUTATIONAL METHOD

## 3.1. INTRODUCTION – DIVISION INTO PHASES

The purpose of the present section is to describe the computational method by which the flow configuration is advanced in time. This is done in general terms, leaving for PART THREE the specification of the computer program which is used to carry out the actual calculation.

It is convenient to express the integral conservation relations, Eqs. 5-7, as finite difference equations over the time step $\Delta t$ and also to decompose the total stress $\sigma_{ij}$ into its deviator and hydrostatic components, according to Eq. 4. This gives, for the increments of total mass (m), momenta ($mu_j$) and energy (mE) within the cell

$$\Delta m = \qquad - \Delta t \int_s \rho u_i n_i ds \tag{8}$$

$$\Delta(mu_j) = -\Delta t \int_s P n_j ds + \Delta t \int_s s_{ij} n_i ds - \Delta t \int_s (\rho u_i u_j) n_i ds \tag{9}$$

$$\Delta(mE) = -\Delta t \int_s P u_i n_i ds + \Delta t \int_s s_{ij} u_j n_i ds - \Delta t \int_s (\rho u_i E) n_i ds \tag{10}$$

Here the terms on the right are divided into increments due to the pressure forces on the cell surface (first column), those due to the stress deviator forces on the cell surface (second column) and the increments (third column) due to the flux of mass, momentum or energy through the surface of the cell. In the computation these three types of contributions are accounted for in distinct phases. Specifically, during each time step all cells are first updated for pressure effects in Phase 1, the effects of the stress deviators are next accounted for in Phase 3 and finally the transport effects are added in Phase 2. In the discussion that follows the calculation of the terms on the right of Eqs. 8-10 are described sequentially starting with Phase 1.

Some preliminary definitions will be helpful. Superscript N on a variable refers to the value of the variable at the beginning of the time step and superscript (N + 1) denotes the value at the end. In this first discussion we consider a typical cell in the interior of the grid, saving until PART 3.6 a discussion of the special conditions which are required at grid boundaries or at the axis of symmetry. For a typical cell, denoted by a value of the index K, the dependent variables for that cell are written P(K), u(K), v(K), I(K), M(K), representing respectively the pressure, radial and axial components of velocity, the specific internal energy and the mass for cell K. The adjacent cells above, below, to the right and left of K will be designated respectively as KA, KB, KR, and KL. Here the terms above, below, right and left refer to a cross section view of the cells, in which the left border is the axis of symmetry with z increasing upward, see Fig. 1. Each cell is, then, the torus obtained by rotating the rectangle (since $\Delta z \neq \Delta r$ in general) about the axis of symmetry. The cells designated by KAL, KAR, LBL and KBR will be referred to in the strain rate calculation discussed in Section 5.

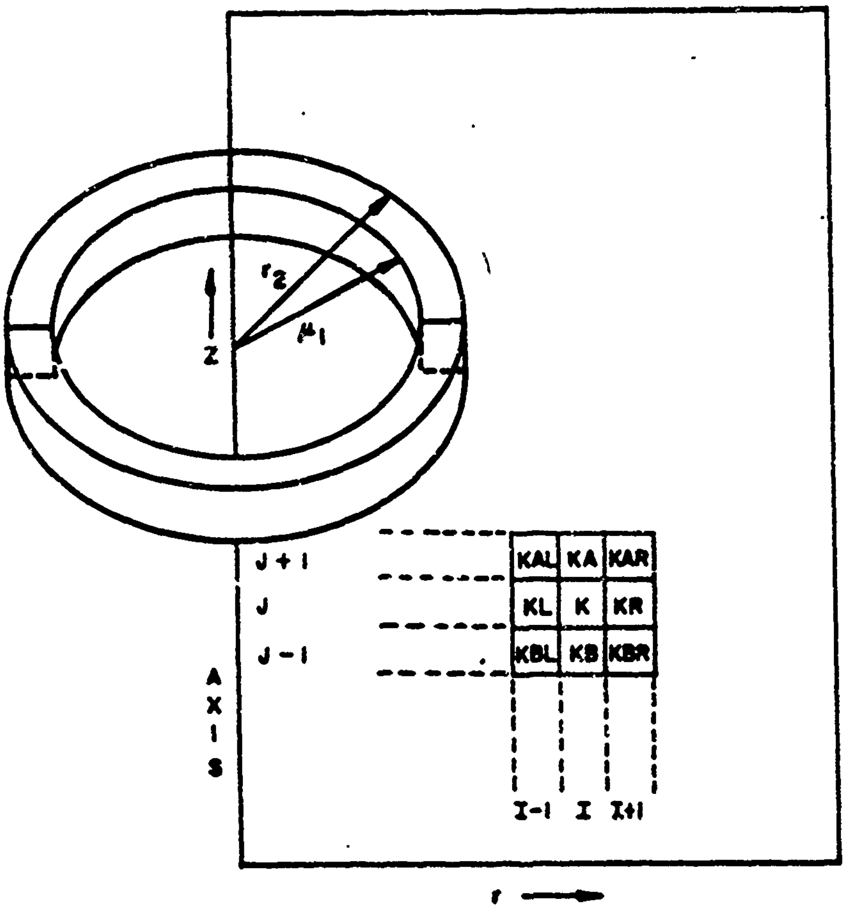

Fig. 1--Grid layout and a typical cell

## 3.2 PHASE 1 – THE EFFECTS OF PRESSURE

### 3.2.1 Continuity Equation, Eq. 8

No contribution in Phase 1.

### 3.2.2 Equations of Motion, Eq. 9

a. Axial Motion. In this case, referring to the pressure integral in Eq. 9, $u_3 = v$ and $n_3 = -1, 0, +1$ are the axial components of the unit normal to the bottom, sides and top of the cell respectively. Equation 9 therefore gives for the Phase 1 contribution

$$\Delta_1(mv) = P_b \, \pi(r_2^2 - r_1^2) \, \Delta t - P_a \, \pi(r_2^2 - r_1^2) \, \Delta t$$

where $r_2$ and $r_1$ are the radii of the outer and inner cell surfaces, respectively, and $P_b$, $P_a$ are the pressure on the bottom and top cell faces. These pressures are obtained from the initial (time N) values of cell pressures by a simple average of the pressures in the adjacent cells:

$$P_b = \frac{P^N(K) + P^N(KB)}{2}$$

$$P_a = P^N(K) + P^N(KA) \ .$$

Making these substitutions gives, for the Phase 1 increment of axial momentum

$$\Delta_1(mv) = \left[\frac{P^N(KB) - P^N(KA)}{2}\right] \pi(r_2^2 - r_1^2) \, \Delta t$$

b. Radial Motion. To arrive at the radial equation of motion it is useful to consider a volume with the full cell dimensions $\Delta z$ and $\Delta r$ in the z and r direction, but with a small angular dimension $\Delta\theta$ instead of $2\pi$, see Fig. 2. Then one can compute the radial motion from Eq. 9 since that motion corresponds to a fixed direction in space. For use in Eq. 9, then, $u_1 = u$, and $n_1 = 1, + 1, \Delta\theta/2, 0, 0$ correspond to the radial components of the unit normals to the inner, and outer surfaces, the two side surfaces and the top and bottom, respectively.

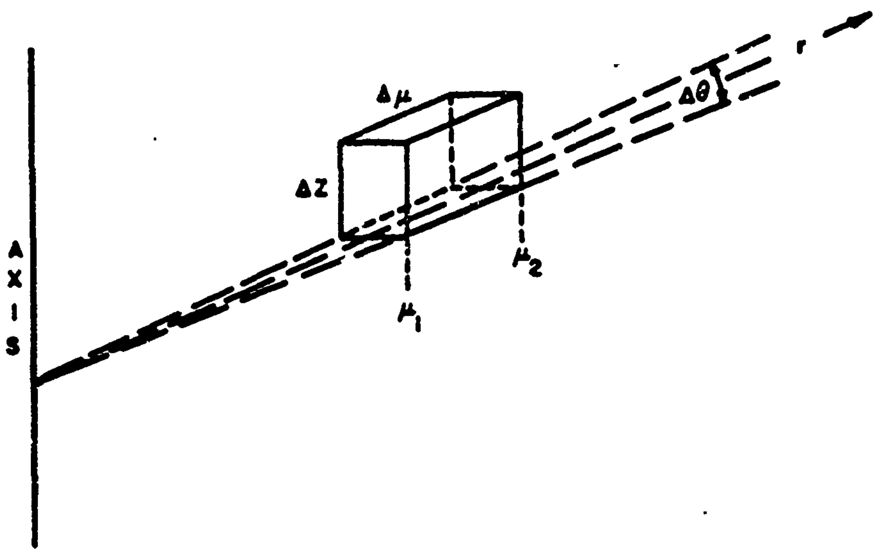

Fig. 2--Element of volume for discussion of radial motion

The pressure-integral contribution in Eq. 9 becomes

$$\frac{\Delta\theta}{2\pi}\Delta_1(\mathrm{mu}) = P_\ell\, r_1\, \Delta\theta\, \Delta z\, \Delta t - P_r\, r_2\, \Delta\theta\, \Delta z\, \Delta t + P_s\, \Delta r\, \Delta z\, \Delta\theta\, \Delta t$$

where $P_\ell$, $P_r$ and $P_s$ are the left, right and side face pressures respectively and are defined in terms of time N cell pressures as follows

$$P_\ell = \frac{P^N(K) + P^N(KL)}{2}$$

$$P_r = \frac{P^N(K) + P^N(KR)}{2}$$

and

$$P_s = (P_\ell + P_r)/2$$

$$= \frac{P^N(KR) + P^N(KL) + 2P^N(K)}{4}$$

In terms of these cell pressures, and using $\Delta r = r_2 - r_1$, the equation for radial motion becomes

$$\Delta_1(mu) = \frac{P^N(KL) - P^N(KR)}{2} 2\pi \left(\frac{r_1 - r_2}{2}\right) \Delta z \; \Delta t$$

c. <u>Energy Equation, Eq. 10</u>. In computing the Phase 1 energy equation we depart somewhat from the standard procedure which is used to compute the other integrals on the right in Eqs. 7-10. Specifically, rather than compute the gain in the total cell energy $m(I + \frac{1}{2}(u^2 + v^2))$ by integrating the pressure forces on the cell surface, the original equation is reformulated to give a volume integral expression for the gain in internal energy, the kinetic energy increment having already been fixed by the preceding calculation of the velocity increments. The resulting equation is preferred because it is a simpler expression for $I$ and because it has been used in most of our calculations and has led to satisfactory results. Starting with the Phase 1 part of Eq. 10,

$$\Delta_1(mE) = - \int_s P u_i n_i ds$$

and since cell mass $m$ is constant in Phase 1 and $E = I + \frac{1}{2} u_i u_i$, one can write

$$\begin{aligned}
\Delta_1(mI) + u_i \, \Delta_1(mu_i) &= - \int_s P u_i n_i ds \\
&= - \int_\tau \frac{\partial}{\partial x_i} (P u_i) d\tau \\
&= - \int_\tau P \frac{\partial u_i}{\partial x_i} d\tau - \int_\tau u_i \frac{\partial P}{\partial x_i} d\tau \\
&= - P \int_\tau \frac{\partial u_i}{\partial x_i} d\tau - u_i \int_\tau \frac{\partial P}{\partial x_i} d\tau
\end{aligned}$$

where $P$ and $u_i$ in the last line are average values over the cell volume. But from the Phase 1 momentum equation

$$\Delta_1(mu_i) = - \int_s P n_i ds$$

or

$$\Delta_1(mu_i) = - \int_\tau \frac{\partial P}{\partial x_i} d\tau$$

so that the last terms on each side of the energy equation cancel and the resulting expression for the gain in internal energy is

$$\Delta_1(mI) = -P \int_\tau \frac{\partial u_i}{\partial x_i} d\tau$$

the difference form is

$$m\Delta I = -\Delta t \; P^N(K) \left(\frac{\partial u_i}{\partial x_i}\right)^{N+\frac{1}{2}} \pi(r_2^2 - r_1^2) \; \Delta z$$

where $(\partial u_i/\partial x_i)^{N+\frac{1}{2}}$ is obtained by averaging the time N (pre-Phase 1) and time (N+1) values, i.e.,

$$\left(\frac{\partial u_i}{\partial x_i}\right)^{N+\frac{1}{2}} = \frac{\left(\frac{\partial u_i}{\partial x_i}\right)^{N} + \left(\frac{\partial u_i}{\partial x_i}\right)^{N+1}}{2}$$

and, for example, the time N value of this divergence is determined from the calculation

$$\frac{\partial u_i}{\partial x_i} = \frac{1}{r} \frac{\partial}{\partial r} (ru) + \frac{\partial v}{\partial z}$$

$$\left(\frac{\partial u_i}{\partial x_i}\right)^{N} = \frac{1}{r_c} \left(\frac{r_r \; u^N(KR) - r_\ell \; u^N(KL)}{2\Delta r}\right) + \frac{v^N(KA) - v^N(KB)}{2\Delta z}$$

in which $r_c = (r_1 + r_2)/2$, $r_r = r_2 + \Delta r/2$, $r_\ell = r_1 - \Delta r/2$ are the radii of cell centers for the central, right and left cells respectively.

This completes the Phase 1 calculation, for a typical cell, of the momentum and internal energy increments due to the pressure forces on the cell. The two momentum increments are used to determine the velocity increments by dividing by cell mass and one has, at the end of Phase 1, values of I(K), u(K), v(K) as updated by Phase 1.

### 3.3. PHASE 3 — THE EFFECT OF SHEAR STRESS

#### 3.3.1. Continuity Equation, Eq. 8

No contribution in Phase 3.

#### 3.3.2. Equation of Motion, Eq. 9

a. Axial Motion. The Phase 3 contribution from Eq. 9 is

$$\Delta_3(mu_3) = \Delta t \int_s s_{i3}n_i ds$$

and for the axial motion

$$u_3 = v$$

Here $s_{i3}n_i$ is the axial (3) component of the total stress on a surface. For a torus with rectangular section, $s_{i3}n_i$ on the various faces is

$s^t_{zz}$ cell top

$-s^b_{zz}$ cell bottom

$s^r_{rz}$ outer cell surface

$-s^\ell_{rz}$ inner cell surface

where zz and rz subscripts denote normal and shear stresses at the top, bottom, right and left surfaces which are indicated by t, b, r and $\ell$ respectively. The equation for axial motion is therefore

$$\Delta_3(mv) = (s^t_{zz} - s^b_{zz}) \pi(r_2^2 - r_1^2) \Delta t + s^r_{rz} 2\pi r_2 \Delta z \Delta t - s^\ell_{rz} 2\pi r_1 \Delta z \Delta t$$

b. Radial Motion. For the radial motion consider the element of mass depicted in Fig. 2. Then in the Phase 3 part of Eq. 9,

$$\Delta_3(mu_1) = \Delta t \int_s s_{i1}n_i ds$$

we have

$$u_1 = u$$

The radial components $s_{i1}n_i$ of the stresses on the various faces of the mass element are

$s_{zr}^{t}$ top of mass element

$-\ s_{zr}^{b}$ bottom

$s_{rr}^{r}$ right

$-\ s_{rr}^{\ell}$ left

$-\ s_{\theta\theta}^{\frac{1}{2}\Delta\theta}$ front

$-\ s_{\theta\theta}^{-\frac{1}{2}\Delta\theta}$ back

The mass of the element is $m\Delta\theta/2\pi$ where $m$ is the cell mass. Then

$$\frac{\Delta\theta}{2\pi}\,\Delta_3(mu) = (s_{zr}^{t} - s_{zr}^{b})(r_2^2 - r_1^2)\ \Delta\theta\ \Delta t + s_{rr}^{r}\ r_2\ \Delta\theta\ \Delta z\ \Delta t$$

$$-\ s_{rr}^{\ell}\ r_1\ \Delta\theta\ \Delta t - s_{\theta\theta}\ \Delta z\ \Delta r\ \Delta\theta\ \Delta t$$

or, multiplying by $2\pi/\Delta\theta$, the equation for radial motion is

$$\Delta_3(mu) = 2\ell\ \Delta t\ [\tfrac{1}{2}(s_{zr}^{t} - s_{zr}^{b})(r_2^2 - r_1^2) + s_{rr}^{r}\ r_2\ \Delta z - s_{rr}^{\ell}\ r_1\ \Delta z - s_{\theta\theta}\Delta z\Delta r]$$

### 3.3.3. Energy Equation, Eq. 10

In the Phase 3 term from Eq. 10,

$$\Delta_3(mE) = \Delta t \int_s s_{ij}u_jn_i ds \qquad ,$$

$s_{ij}u_jn_i$ is the work rate per unit surface area, which for the various faces of the torus, is

$(s_{zz}^{t}\ v^{t} + s_{zr}^{t}\ u^{t})$ cell top

$-\ (s_{zz}^{b}\ v^{b} + s_{zr}^{b}\ u^{b})$ cell bottom

$$(s_{rz}^{r}\ v^{r} + s_{rr}^{r}\ u^{r})\ \text{outer cell surface}$$

$$(s_{rz}^{\ell}\ v^{\ell} + s_{rr}^{\ell}\ u^{\ell})\ \text{inner cell surface}$$

where t, b, r, $\ell$ denote stresses and velocities at the top, bottom, right and left cell faces respectively. The calculation of these stresses from the material constitutive relations is discussed in Section 5 and the interface velocities are determined from a simple average of the time N velocities in the two cells, e.g.

$$v^{t} = \frac{v^{N}(K) + v^{N}(KA)}{2}$$

$$u^{\ell} = \frac{U^{N}(K) + u^{N}(KL)}{2}$$

The equation for the Phase 3 change in total cell energy is

$$\Delta_3(mE) = (s_{zz}^{t}\ v^{t} + s_{zr}^{t}\ u^{t} - s_{zz}^{b}\ v^{b} - s_{zr}^{b}\ u^{b})\ \pi(r_2^2 - r_1^2)\ \Delta t$$

$$+ (S_{rz}^{r}\ v^{r} + s_{rr}^{r}\ u^{r})\ 2\pi\ r_2\ \Delta z\ \Delta t - (s_{rz}^{\ell}\ v^{\ell} + s_{rr}^{\ell}\ u^{\ell})\ 2\pi\ r_1\ \Delta z\ \Delta t$$

This completes the Phase 3 calculation, for a typical cell, of the momentum and total energy increments due to the deviator stresses acting on the cell. The two momentum increments are used to determine the velocity increments by dividing by cell mass. This fixes the Phase 3 change in cell kinetic energy $\frac{1}{2}u_i u_i$ so that the internal energy (I) can be calculated using the updated value of total energy $E = I + \frac{1}{2}u_i u_i$. At the end of Phase 3 one therefore has new values of I(K), u(K), v(K) as updated by Phase 3.

## 3.4. PHASE 2 – THE EFFECT OF TRANSPORT

The purpose of this section is to describe how the transport of mass, momentum and energy from cell to cell is accounted for in the code. This is done by calculating the integrals in the last terms of Eqs. 8 to 10. The method is that given previously as Ref. 2 and is a continuous analog of the transport which has been discussed in relation to earlier PIC codes.(7,8)

### 3.4.1. Continuity Equation, Eq. 8

The transport mass is

$$\Delta_2(m) = -\Delta t \int_s \rho u_i n_i ds$$

and is determined for each of the cell faces from

$$\delta m = -\rho^N u_i^N A_i \Delta t$$

where $\rho$ is the density of the cell from which the mass moves (donor cell), $A_i$ is the area of the face and $u_i^N$ is an interpolated value of the velocity component normal to $A_i$ representing approximately the velocity at the interface at the end of the time step. For example, considering cell K and the cell KA above, one has

$$v_i^N = \frac{\frac{1}{2}[v^N(K) + v^N(KA)]}{\left[1 + \frac{v^N(KA) - v^N(K)}{\Delta z} \Delta t\right]}$$

The calculated transport masses are subtracted from the donor cell mass and added to the acceptor cell mass. This updating is done, however, after the transport terms have been calculated, so that all of the transport terms are computed using time N quantities.

### 3.4.2. Equation of Motion, Eq. 9

a. Axial Motion. The term in Eq. 9 for axial momentum transport is

$$\Delta_2(mu_3) = -\Delta t \int_s (\rho u_3 u_i) n_i ds .$$

At each face of the cell the transport specific momentum, $u_3$, is taken to be the axial velocity of the cell from which the mass moves (donor cell, index KD), i.e.

$$u_3 = v^N(KD) .$$

Since the various faces of the cell have different donor cells it is convenient to express the momentum transport for each face

$$\delta(mv) = v^N(KD) \delta m$$

where

$$\delta m = -\rho^N u_i^N A_i \Delta t$$

is the mass which is transported across the interface, as given in the preceding mass transport calculation. Note that $\delta(mv)$ and $\delta m$ are the momentum and mass transports in either the axial or radial directions, depending on which type of interface is being computed.

b. Radial Motion. Again we have from Eq. 9

$$\Delta_2(mu_1) = -\Delta t \int_s (\rho u_i u_1) n_i \, ds$$

and, by analogy with the axial case, the equation for the transport of radial motion across an interface is

$$\delta(mu) = u^N(KD) \, \delta m$$

where $u^N(KD)$ is the time N velocity of the donor cell and $\delta m = -\rho^N u_i^N A_i \Delta t$ is the mass which is transported across the interface in question, as computed in 3.4.1 above.

### 3.4.3 Energy Equation, Eq. (10)

The Eq. (1) expression for the transport of energy is

$$\Delta_3(mE) = -\Delta t \int_s (\rho u_i E) n_i \, ds \ .$$

To evaluate this integral, the transported specific energy is taken to be that of the donor cell KD, i.e.

$$E_D \equiv I^N(KD) + \frac{1}{2} \left[ \left(u^N(KD)\right)^2 + \left(v^N(KD)\right)^2 \right]$$

and the total energy which is transported across a given interface is therefore the product of this specific energy and the associated transport mass which was computed above in 3.4.1.,

$$\Delta_3(mE) = E_D \, \delta m$$

Once the mass, momentum and energy transports are known for all faces of the cell, the cell quantities can be updated for these effects. New cell velocities are determined by dividing the new momenta by updated cell mass. This fixes the new kinetic energy so that the internal energy can be calculated from the known total energy. At the end of Phase 2 one has final values of u(K), v(K), I(K), M(K), the cell velocities, specific internal energy and mass.

## 3.5. CELL PRESSURES AND TIME STEP FOR NEXT CYCLE

New cell pressures, to be used in the next time step, are computed from an equation of state giving cell pressure as a function of density and specific internal energy within the cell. Such an equation of state is the subject of Section 4.

For stability of the solution the new time-step is taken to be less than the time for either a sound wave or a mass element to cross a cell. In most problems the actual time step is some factor, 0.4 to 0.7, of this minimum transit time.

## 3.6. SPECIAL FEATURES OF THE COMPUTATION

### 3.6.1. Grid Boundaries and Axis

Additional specification is required for cells which border the grid boundaries or axis of symmetry, because necessary quantities are not defined for neighbor cells which would be outside the grid.

The code provides for a transmittive boundary at the top and right, an option of a transmittive or reflective boundary at the bottom and a reflective boundary at the axis. Boundary conditions for border cells are then derived by assuming (fictional) neighbors cells outside the grid. For transmittive boundaries the flow variables are the same in the fictional cell as in the border cell, and for reflective boundaries the state is assumed to be the same except that the velocity component normal to the boundary has opposite sign.

### 3.6.2. Free Surface Motion

Unless additional provisions were made, the preceding method would result in a diffusion of the free surface over several cell dimensions. To avoid this, a revised calculation is made to determine transport masses at free surfaces, as described in the next two paragraphs.

Consider, for example, the upward motion of a free surface, from the cell K which contains it to the empty cell KA above. If the density of the average cell K is less than the normal and if the specific internal energy of both cell K and the cell below are less than that required to bring the material to its vaporization point, then the transport mass from K to KA is set to zero. Otherwise, the mass transported from K to KA is given by $\delta m = \rho(K)\ v(K)\ A\ \Delta t$ where A is the area of the interface. This procedure amounts to requiring that cell K be filled before material is transported to KA, if the material is condensed. The same procedure is used for the motion of a free surface into empty cells to the right, left or downward.

A similar calculation is made for a receding free surface, i.e., one which empties the cells from which it passes. Consider the case similar to the one above, except that the motion is downward, so that one is concerned with evaluating the transport mass from K to KB. If either K or KB has specific internal energy greater than that required to bring the material to its vaporization point, the normal mass transport calculation is made, using the donor cell (K) density and an interpolated velocity. But if both cells are cold, the mass transported is $\delta m = \rho(KB)\ v(KB)\ A\ \Delta t$. Here the use of the generally higher density $\rho(KB)$ causes a greater transport mass, making it possible to evacuate free surface cells. In the unmodified method some residual mass would always be left in an evacuating cell. With the existing method the cell may overempty, but this is immediately corrected should the cell mass become negative.

### 3.6.3. Rezone

A rezone subroutine can be triggered by mass motion out of the right or top grid boundaries. Four cells are combined into one, starting at the lower left corner ($z = 0$, $r = 0$) of the grid and new cells are added at the top and right. The total number of cells is held constant, as well as their shape.

### 3.6.4. Tracer Points

A system of "tracer points" can be deployed in the initial material configuration and these points are transported with local material velocity during the computation. While these points do not enter the actual solution to the flow equations, their dispositions at various times can give quick and valuable insight into the meaning of the solution.

### 3.6.5. Variable Zoning

Although the discussion has proceeded with no special reference to variable zoning, the current version of OIL-RPM reported in PART THREE is able to compute problems in which the zone size is variable. If constant zones are not specified, the cell sizes must be supplied as a part of the SETUP deck. It is possible to call for variable cell size in one direction and constant in the other.

The zones must be selected so that the discontinuities in size between adjacent cells are not excessive and the aspect ratio of the cells are not too extreme. It was found that an initially spherical explosion loses its symmetry in the course of a calculation when the ratio of the cell edges is greater than four to one, and that satisfactory symmetry is obtained when the ratio is two to one. Cell size variations are usually held to less than 10 percent between adjacent cells. This resulted in good accuracy in a test problem.

## 4. EQUATION OF STATE FOR THE CALCULATION OF PRESSURE

Since the flow equations contain the pressure, p, the density, $\rho$, and the specific internal energy, I, it is natural to make use of an equation of state relating these particular variables. A description of such an equation $p(I,\rho)$ developed for hypervelocity impact calculations is given by Tillotson.(9) His formulation fits Thomas-Fermi data at high pressures (10 megabars and above), experimental shock-wave measurements at more moderate shock pressures, and at low density and high energy it describes a material which behaves in the limit as an ideal gas. This is done by means of an equation of the form

$$p = p_S(I,\rho) = G(I,\rho)\, I\rho + A\mu + B\mu^2$$

where

$$\mu = \eta - 1, \qquad \eta = \rho/\rho_0$$

and

$$G(I,\rho) = a + \frac{b}{\dfrac{I}{E_0\,\eta^2} + 1} \, .$$

At high internal energy and low density the equation of state has the form

$$p = p_G(I,\rho) = aI\rho + \left\{ \frac{bI\rho}{\dfrac{I}{E_0\,\eta^2} + 1} + A\mu \; e^{-\beta\left(\frac{1}{\eta} - 1\right)} \right\} e^{-\alpha\left(\frac{1}{\eta} - 1\right)^2}$$

The equation of state described by Tillotson is used in a slightly modified form in the current program. The regime in which material is neither vaporized fully ($I < I''$) nor completely condensed ($I > I'$) is computed by weighting the two expressions above. Specifically, if $I' < I < I''$ then

$$p = \frac{(I-I')\, p_S + (I''-I)\, p_G}{I'' - I'}$$

Here $I'$ is the energy of the material which just brings it to the vapor temperature and $I''$ includes the additional energy to complete the transition to the vapor state.

This formulation allows material to condense from the vapor state into the "dust" state in a continuous manner. By "dust", here, is meant a state where the internal energy is inadequate to bring material to the vapor temperature but so expanded that it cannot support pressure.

In the notation above I is used to denote specific internal energy, as in the other portions of this report. Tillotson,(9) however, uses E, and in portions of the program documented in PART THREE, "E" may denote specific internal energy.

Material is allowed to support tensions (negative pressures) in the current version of the program. The maximum expansion is specified by AMDM. If the material is cold ($I < I'$) and $\eta <$ AMDM the pressure is set to zero. Then the material is thought of as cracked, with the cracks smaller in size than a cell, or as dust, depending on the density of the material. AMDM is typically a number like 0.97. For small expansions the expressions above for pressure reduce approximately to

$$p = G_0 I\rho + A\mu ,$$

where $G_0$ is Gruneisen's ratio.

Thus, for aluminum, assuming the first term is negligible, we would find $p = -22.5$ kilobars using the value $A = 0.75$ megabars given by Tillotson.

A table of constants appropriate for representing a variety of metals is given in PART THREE. The information for metals is taken from the Tillotson report and for geologic materials it is taken from a report by Allen.(10)

Some general remarks can be made regarding the above equation of state.

a. The pressure is continuous in $\rho$ and I in the various regions and across transitions between the regions.*

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* We are indebted to Caroti of General Electric for pointing out to us an error in an earlier version. Specifically, isentropes computed from the equation of state given in Ref. 9 can be discontinuous in pressure at the condensed-vapor transition. The correction of this error has lead to significantly smoother solutions to several applications of RPM.

b. No equation of state formulation is ideally suited to all applications. The present one is especially suited to situations in which the material experiences a strong shock (say tens of megabars) and subsequently expands. Examples are the hypervelocity impact problem and certain ground shock applications. For quite different applications, other equation of state formulations should be considered. For example, problems involving cold highly compressed states ($\rho/\rho_0 > 3$, not achieved in a single shock) should be computed using an equation of state which is formulated with such states in mind. Also simpler equations of state may be desired in some cases. An example is ordinary shock wave hydrodynamics at pressures less than a megabar, where several simpler forms have been widely used in past years.

It is expected that other users of OIL-RPM may want to include additional equations of states. No special difficulties are envisioned in such extensions.

# 5. CONSTITUTIVE EQUATIONS FOR THE CALCULATION OF DEVIATOR STRESS

In Section 3.3 the effect of shear stresses on the calculation of velocity and internal energy increments (through the conservation equations) was discussed. The total stress was broken up into an isotropic component (pressure) and a deviator stress. The calculation of pressures from density and internal energy was then discussed in Section 4. The finite difference technique for calculating the deviator stresses from the velocity field will be the subject of this section. It is based on the rigid-plastic model relating deviator stress and deviator strain rate discussed in PART ONE. The motivation for selecting the rigid-plastic model (primarily its simplicity) among the possible bases for a constitutive equation was also described there.

## 5.1. FINITE DIFFERENCE APPROXIMATIONS

Deviator stresses act on each face of a cell to accelerate the mass it contains, as sketched in Fig. 3. A tabulation of these stresses is given below, and in the table the relation of the current notation to that used in Section 3, is also indicated. This current notation is consistent with the FORTRAN symbols used in the program in PART THREE of this report.

TABLE 5.1

NOTATION FOR STRESSES ACTING ON A CELL

| Area | Normal | Tangent | Hoop |
|---|---|---|---|
| Top | SNT = $S^t_{zz}$ | STT = $S^t_{zr}$ | --- |
| Right | SNR = $S^r_{rr}$ | STR = $S^r_{zr}$ | --- |
| Left | SNL = $S^\ell_{rr}$ | STL = $S^r_{zr}$ | --- |
| Bottom | SNB = $S^b_{zz}$ | STB = $S^b_{zr}$ | --- |
| Cross Section | --- | --- | Hoop |

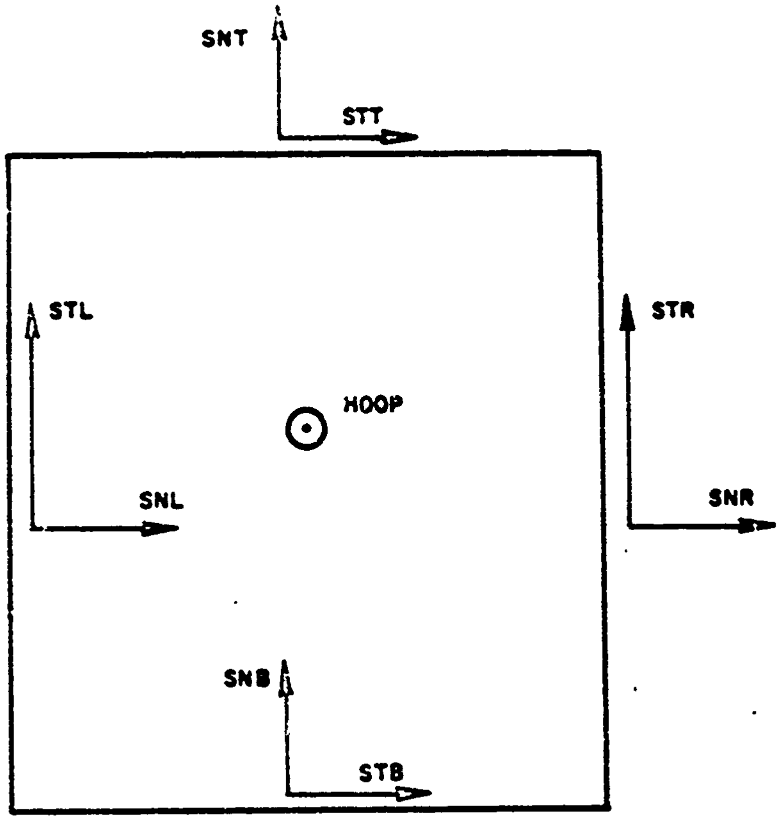

Fig. 3--Deviator stresses used in the Phase 3 calculation

The notation in the table is related to the more formal subscript notation of PART ONE by the equations

$$S_{11} = S_{rr} , \quad S_{13} = S_{rz} , \quad S_{22} = S_{\theta\theta} , \quad S_{33} = S_{zz} .$$

The required deviator stresses are computed from the strain rates by means of the relation

$$S_{ij} = Y \sqrt{2/W} \; e_{ij}$$

indicated in PART ONE, where Y is the yield strength in simple shear,

$$e_{ij} = \epsilon_{ij} - \theta\delta_{ij} , \qquad \theta = \epsilon_{ii}/3$$

and

$$W = e_{ij}\, e_{ij} .$$

The strain-rate tensor in cylindrical coordinates is given by the matrix

$$(\epsilon_{ij}) = \begin{pmatrix} u_r & 0 & \frac{1}{2}(u_z+v_r) \\ 0 & u/r & 0 \\ \frac{1}{2}(u_z+v_r) & 0 & v_z \end{pmatrix}$$

where the subscripts r and z denote differentiation with respect to the subscripted variable. Expressions for θ and W are obtained by substitution of the matrix elements into the expressions above.

$$\theta = \frac{1}{3}(u_r + \frac{u}{r} + v_z)$$

$$W = u_r{}^2 + v_z{}^2 + (u/r)^2 + \frac{1}{2}(u_z + v_r)^2 - 3\theta^2 .$$

The velocity gradients used in calculating the stresses are determined in such a way that the velocities of the cells adjoining each interface enter into the calculation in a symmetrical manner. Details of the differencing are indicated in Table 5.2. The cell size is DRV(I) in the radial direction, DZV(J) in the axial direction,

## TABLE 5.2

## CALCULATION OF VELOCITY GRADIENTS

Top-centered Variables

$$\frac{\partial u}{\partial z} = \frac{u(KA) - u(K)}{DZV(J)} \qquad \frac{\partial u}{\partial r} = \frac{\frac{1}{2}(u(KR) + u(KAR)) - \frac{1}{2}(u(KL) + u(KAL))}{2DRV(I)}$$

$$\frac{\partial v}{\partial z} = \frac{V(KA) - v(K)}{DZV(J)} \qquad \frac{\partial v}{\partial r} = \frac{\frac{1}{2}(v(KR) + v(KAR)) - \frac{1}{2}(v(KL) + v(KAL))}{2DRV(I)}$$

$$\frac{u}{r} = \frac{u(KA) + u(K)}{2R(I)}$$

$$DZV(J) = \frac{1}{2}(DZ(J+1) + DZ(J)), \qquad 2DRV(I) = \frac{1}{2}DR(I-1) + DR(I) + \frac{1}{2}DR(I+1)$$

Right-centered Variables

$$\frac{\partial u}{\partial z} = \frac{\frac{1}{2}(u(KA) + u(KAR)) - \frac{1}{2}(u(KBL) + u(KBR))}{DZV(J)} \qquad \frac{\partial u}{\partial r} = \frac{u(KR) - u(K)}{DRV(I)}$$

$$\frac{\partial v}{\partial z} = \frac{\frac{1}{2}(v(KA) + v(KAR)) - \frac{1}{2}(v(KB) + v(KBR))}{DZV(J)} \qquad \frac{\partial v}{\partial r} = \frac{v(KR) - v(K)}{DRV(I)}$$

$$\frac{u}{r} = \frac{u(K) + u(KR)}{R(I) + R(I+1)}$$

$$DRV(I) = \frac{1}{2}(DR(I) + DR(I+1)), \qquad DZV(J) = DZ(J)$$

Cell-centered Variables

$$\frac{\partial u}{\partial z} = \frac{u(KA) - u(KB)}{2DZV(J)} \qquad \frac{\partial u}{\partial r} = \frac{u(KR) - u(KL)}{2DRV(I)}$$

$$\frac{\partial v}{\partial z} = \frac{v(KA) - v(KB)}{2DZV(J)} \qquad \frac{\partial v}{\partial r} = \frac{v(KR) - v(KL)}{2DRV(I)}$$

$$\frac{u}{r} = \frac{u(K)}{R(I)}$$

$$2\ DZV = \frac{1}{2}DZ(J+1) + DZ(J) + \frac{1}{2}DZ(J-1)$$

$$2DRV = \frac{1}{2}DR(I+1) + DR(I) + \frac{1}{2}DR(I-1)$$

and, as suggested by the notation, these may vary from cell to cell. Expressions for DRV(I) and DZV(J) in terms of cell dimensions DR(I) and DZ(J) are included in the table. DR(I) and DZ(J) are abbreviated as DR and DZ in some of the following equations for brevity of notation.

Values for the left and bottom deviator stresses do not have to be determined separately since they are calculated as the right and top deviator stresses for the cells to the left and below respectively. In the finite difference notation described in the preceeding paragraphs the equations of Section 3.3 become

$$\Delta_3(mv) = 2\pi\Delta t\,[(SNT - SNB)\cdot R\cdot DR + (STR\cdot R^r - STL\cdot R^\ell)\cdot DZ]$$

and

$$\Delta_3(mu) = 2\pi\Delta t\,[R^r\cdot DR(STT\text{-}STB) + DZ(SNR\cdot R^r - SNL\cdot R^\ell) - HOOP\cdot DR\cdot DZ]$$

where R is the coordinate of the cell center and $R^r$ and $R^\ell$ are coordinates of the right and left edges:

$$R^r = R + \tfrac{1}{2}DR, \qquad R^\ell = R - \tfrac{1}{2}DR\ .$$

To calculate the change in internal energy in a cell it is noted that the change in its total energy is determined by the stresses acting on its boundary, and the change in kinetic energy is determined by the change in velocity, which in turn is obtained from the momentum equations. The difference of the changes in total and kinetic energy in the change in internal energy. The change in internal energy of a cell due to pressure is accounted for in Phase 1, and the change due to the deviator stresses, which may be thought of as the plastic work, is accounted for in Phase 3. The Phase 3 change in internal energy is computed in several parts, viz,

$$\Delta_3(mI) = (A+B)\,\Delta t - [(u+\tfrac{1}{2}\Delta_3 u)\,\Delta_3 u + (v+\tfrac{1}{2}\Delta_3 v)\,\Delta_3 v]$$

where

$$A = 2\pi R\cdot DR\left\{\tfrac{1}{2}(u(K) + u(KA))\cdot STT + \tfrac{1}{2}(v(K) + v(KA))\cdot SNT - \tfrac{1}{2}(u(K) + u(KB))\cdot STB - \tfrac{1}{2}(v(K) + v(KB))\cdot SNB\right\}$$

and

$$B = 2\pi\, DZ \left\{ \frac{1}{2} R^r \cdot (u(KR) + u(K)) \cdot SNR + \frac{1}{2} R^r\, (v(KR) + v(K)) \cdot STR - \frac{1}{2} R^{\ell} (u(K) + u(KL)) \cdot SNL - \frac{1}{2} R^{\ell} (v(K) + v(KL)) \cdot STL \right\}$$

The plastic work done in a single cycle in a single cell is $\Delta_3(mI)$. It is positive in principle, though not necessarily in the calculation, as a result of the finite time step. The sum of the plastic work done on each cell in each cycle is accumulated into a grand total which is printed out at each of the edit times. This is the "plastic work" exhibited in the edit prints.

It is possible for the change in velocity in a single cycle due to plastic stresses to be so large that the velocity profile changes curvature. This difficulty can be largely corrected by subcycling. Specifically, the time step for Phase 3, is divided into N steps, where

$$\Delta_1 t = N \frac{2\Delta t}{N(N+1)}, \quad \Delta_2 t = (N-1) \frac{2\Delta t}{N(N+1)}, \quad \dots, \quad \Delta_N t = \frac{2\Delta t}{N(N+1)}$$

The number of time steps (CYCPH3) is left to the discretion of the user, but experience has shown that 4 is a good choice.

The problems that the OIL-RPM code has been called upon to calculate have involved shocks diverging out from either an impact or an explosion. In either case a very significant improvement is obtained by preventing the Phase 3 calculation from affecting the flow outside the shock. To do this the shock has to be located, at least in an approximate manner. This is done by seeking out the location of the first pressure maximum in each column of cells. The result is used to update the JPM(I) array, which gives the J index of the cell with the Pressure Maximum in column I. The updating of JPM(I) is done in the subroutine CDT which determines the time step. The JPM(I) have to be halved when rezoning, and that is done in the subroutine "REZONE."

## 5.2. VARIATIONS IN YIELD STRENGTH

Experiments (11)(12) have shown that yield strength depends on pressure and temperature. Although an appropriate set of constitutive equations fully describing these effects is not available, the calculation of Phase 3 attempts to account for them by allowing the flow stress, Y, to vary according to the relation

$$Y = (Y_0 + Y_1\mu + Y_2\mu^2)(1-I/E_0)$$

where

$$\mu = \frac{\rho}{\rho_0} - 1 .$$

I is the specific internal energy and $E_0$ is the energy which raises the material to the melting point. If either factor is negative the yield strength is set to zero. This formula is not intended as an accurate representation of the physical behavior of materials, but was included in the program so that the importance of yield strength variations could be estimated.

Although no formal report has been written, it seems appropriate to mention here a calculation in which the second factor in the expression above for Y was set equal to unity. The calculation otherwise duplicated the standard impact crater problem reported in Ref. 14. The effect was to decrease the crater depth at 14 μsec from 1.16 to 1.11 cm. At that time the rate of change of depth is down to $10^3$ cm/sec and thus its growth is essentially terminated. In a second comparison it was found that setting the first factor to unity made the crater depth at 14 μsec 1.18 cm rather than the 1.16 cm computed in the standard problem.

To summarize, the effect of yield strength variations can be accounted for in an approximate manner by choosing appropriate values for $Y_1$, $Y_2$ and $E_0$, but this does not seem to influence crater size in the first approximation. $E_0$ can be found from handbooks as the internal energy at the point where the yield strength goes to zero, and this can be taken roughly as the internal energy at melting in the absence of detailed information. $Y_1$ and $Y_2$ can be estimated from the relation, $Y = Y_0 + \alpha P$, which is valid at low pressures. The value of $\alpha$ is about 0.07 for metals and near unity for geological materials.

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