CONF-880638--1

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

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LA-UR--88-1691

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DE88 010950

SUBMITTED TO International Conference on Computational Physics,
Beijing, China, 1-5 June, 1988

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MATERIAL VOID OPENING COMPUTATION USING PARTICLE METHOD

by

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ABSTRACT

When performing the calculation of material flow in two dimensional Eulerian coordinates, one always encounters the difficulties of modeling the void opening due to material failure such as fracture, spallation, or phase change. The present studies use one type of particle to represent the material and another type for the void space. According to the flow conditions, the void space may grow with crack propagation or may be recombined with the void space closed up when the volume decreases. The penetration of a copper rod into, and eventually through a steel plate, is calculated using the present code.

I. INTRODUCTION

One of the well-known difficult problems in computing the impact or penetration phenomena is the modeling of the void opening due to material failure such as fracture or spallation. The present studies use one type of particle to represent the material and another type for the void space. According to the flow

conditions, the void space may grow with crack propagation or may be recombined with the void space closed up when the volume decreases. Particles may be added to or removed from the cell, dependent on whether the cell is partially void or not. Essentially, the free surfaces, that is, material surfaces adjacent to void or vacuum, are tracked by particles while pure material zones are computed without particles.

The particle-in-cell (PIC) and operator splitting methods are used to solve the hydro-plastic-elastic flow in two dimensional Eulerian r - z coordinates. By applying the operator splitting method, the governing set of cylindrical equations is split in radial and axial directions. Then a separate calculation is performed in each direction. The order of this calculation is alternated for each time advancement to maintain the accuracy of the one dimensional procedure. For the PIC method, the Lagrangian quantities at the new step are computed first and then followed by the particle transport. In the second phase, particles are transported for the interfacial zones (either material-material or material-void interfaces) with particle portions of momentum, internal energy, and stresses. These transported quantities are then summed up for each cell and new quantities at the new time step are calculated.

The penetration of a copper rod into, and eventually through the steel plate, is calculated using the present code. Cratering and material fracture, as well as spallation of the steel, demonstrate the stable calculations of the present numerical scheme.

II. CALCULATION PROCEDURE AND VOID OPENING CHECK

An operator splitting method is applied here. The governing set of cylindrical equations is split in the radial and axial directions. A separate calculation is performed in each direction. The order of this calculation is alternated for each time advancement to maintain the accuracy of the one-dimensional procedure. The sequence of steps in a computation step is presented briefly below.

2.1 Summary of equations in the axial direction

Mass:

$$\rho_t = -\nu \rho_z - \rho \nu_z \quad . \quad (1)$$

Momentum:

$$u_t = -\nu u_z + \frac{1}{\rho} \sigma_z^{rz} \quad . \quad (2)$$

$$\nu_t = -\nu \nu_z + \frac{1}{\rho} \sigma_z^{zz} \quad . \quad (2a)$$

Energy:

$$I_t = -u I_r + \frac{1}{\rho} \{ \sigma^{zz} \nu_z + \sigma^{rz} u_z \} \quad . \quad (3)$$

EOS:

Pressure:

$$P = g(\rho, I) \quad .$$

Elastic regime:

$$S_t^{rr} = -\nu S_z^{rr} + 2G[-\frac{1}{3}\nu_z] \quad , \quad (4)$$

$$S_t^{zz} = -\nu S_z^{zz} + 2G[\frac{2}{3}\nu_z] \quad . \quad (4a)$$

$$S_t^{rz} = -\nu S_z^{rz} + 2G[\frac{1}{2}u_z] \quad , \quad (4b)$$

and

$$S^{\theta\theta} = -(S^{rr} + S^{zz}) \quad . \quad (4c)$$

Plastic regime:

$$S_{ij}^p = (S_{ij}^e) - \left\{ \frac{3G}{(\bar{Y}^0)^2} \right\} \dot{W} S_{ij}^e \quad (5)$$

where ρ is the material density, t is the time, u and v are the velocities in r - and z -directions. Respectively, σ_{ij} is the stress tensor, I is the specific internal energy, P is the pressure, S_{ij}^e is the deviatoric stress tensor, G is the shear modulus, $(S_{ij}^e)_e$ is the elastic component, and $\dot{W}$ is the plastic work/unit volume.

2.2 Lagrangian phase

Based on known quantities at n th time-step (denoted by superscript n), Lagrangian quantities at $(n+1)$ th time-step are computed (denoted by a wiggle). A bar on the top of a variable indicates the time average, e.g., $\bar{u} = 0.5(u^n + \bar{u})$.

$$\bar{u} = u^n + \delta t (\sigma_z^{rz} / \rho)^{n+1/2} = u^n + \frac{\delta t}{\rho^n} [(\sigma^{rz})^{n+1/2}]_z \quad (6)$$

$$\bar{v} = v^n + \delta t (\sigma_z^{zz} / \rho)^{n+1/2} = v^n + \frac{\delta t}{\rho^n} [(\sigma^{zz})^{n+1/2}]_z \quad (6a)$$

$$\begin{aligned} \bar{I} &= I^n + \delta t \left(\frac{1}{\rho} \sigma^{zz} v_z + \frac{1}{\rho} \sigma^{rz} u_z \right)^{n+1/2} \\ &= I^n + \frac{\delta t}{\rho^n} \left\{ (\sigma^{zz})^{n+1/2} \bar{v}_z + (\sigma^{rz})^{n+1/2} \bar{u}_z \right\} \quad (6b) \end{aligned}$$

$$f^{n+1/2} = f^n + \frac{\delta t}{2} (f_t + v f_z) \quad (7)$$

and

$$p^{n+1/2} = g(\rho^{n+1/2}, I^{n+1/2}) \quad (7a)$$

In the elastic regime

$$\tilde{S}^{rr} = (S^{rr})^n + \delta t \left(-\frac{2}{3}G\nu_z\right)^{n+1/2} = (S^{rr})^n + \delta t \left\{ -\frac{2}{3}\overline{G}\nu_z \left(1 - \frac{\delta t}{2}\nu_z\right) \right\} \quad (8)$$

$$\tilde{S}^{zz} = (S^{zz})^n + \delta t \left(\frac{4}{3}G\nu_z\right)^{n+1/2} = (S^{zz})^n + \delta t \left\{ \frac{4}{3}\overline{G}\nu_z \left(1 - \frac{\delta t}{2}\nu_z\right) \right\} \quad (8a)$$

and

$$\tilde{S}^{rz} = S^{rz})^n + \delta t (Gu_z)^{n+1/2} = (S^{rz})^n + \delta t \left\{ \overline{G}u_z \left(1 - \frac{\delta t}{2}\nu_z\right) \right\} \quad (8b)$$

In the plastic regime

$$(\tilde{S}^{ij})_p = (\tilde{S}^{ij})_e - \delta t \frac{3G\dot{\gamma}}{(\gamma^0)^2} (S^{ij})^{n+1/2} \quad (9)$$

where $(\tilde{S}^{ij})_e$ = elastic portion given by Eqs. (4) to (4c).

2.3 Remapping and void opening

After the Lagrangian phase calculation, we have $\tilde{u}$, $\tilde{\nu}$, $\tilde{I}$ and $\tilde{S}^{ij}$ at each cell. Consistent with these, temporary values of momentum and internal energy are assigned to cell (i) as below.

$$\text{Momentum} = M_i \tilde{u}_i$$

and

$$\text{Internal energy} = M_i \tilde{I}_i \quad (10)$$

where M_i = Mass of cell (i).

For a pure material cell, i.e., only one type of material is presented, we use the fluid volume transport calculations without introducing any particles. If a cell contains two or more materials or void, then a total of 64 particles are created for each material or void in the mixed cell. The particles are transported with the average velocity, for example, in the radial direction,

$$\bar{u} = \frac{1}{2}(u^n + \bar{u}) \quad .$$

Each particle carries with it a fraction in proportion to the particle mass of dynamic and state quantities as defined by Eq. (10). In the case of void, the mass is zero. A particle can cross no more than one cell during a time step as limited by the stability requirement. A more detailed description of the particle transport and remapping are given in Ref. (1). After the particle transport, total changes in momentum, energy, and stresses are calculated for each cell by summing the contributions of the particles. We use a particle treatment for cell i under the following conditions (see Fig. 1): (1) if cell i is multi-material or is partially filled; (2) if cells i and $i-1$ are both pure material (no void) but not the same kind; (3) if cells i and $i+1$ are both pure material (no void), but not the same kind; (4) if cell i , a donor cell, is pure and the acceptor cell, for example cell $i+1$, is a multi-material or partially filled zone. For those cells that do not meet any of the above mentioned conditions will be treated using ordinary finite difference without any particles. The computation on or around a spalled cell can vary widely depending on the accuracy desired for spall. Mathematically, the material failure creates a discontinuity within the computational domain. Therefore, for a rigorous treatment, a proper interface condition (possibly jump condition) has to be established across a spalled cell. Basically, spall or fracture has Lagrangian characteristics and, to resolve it in an Eulerian mesh system, requires a special spall logic. For the present computation, a rather simple scheme is suitable for the particle code. When a material is spalled, a void region is created and located at the cell center with a minimum number of 16 particles. Then, for subsequent time steps, this is convected with average velocities. Pressure and stresses are set to be zero at this point. This is essentially the same as introducing a rectangular void at the cell center. The void region has an initial volume based on the equation-of-state and may grow later. If the center of a spalled cell (i,j) as shown in Fig. 1

is moved to a new location (i', j') , the specific volume v for (i', j') is computed by averaging values in dotted cell. When the specific volume is less than a specified number, the dotted cell is assumed to be recombined. The particle code in its present form will not follow a fractured surface exactly. Rather, the density of the fractured cell will be computed by a volume average using the actual volumes of material and void in the cell. The propagation of a crack or a material separation will be resolved in this fashion. Currently, particles are created in the fractured cell and assigned an identification number of 31 for fractured void space (see Fig. 2).

Fig. 1. Old and new centers of a spalled cell.

Fig. 2. Material number 31 is assigned to a spalled or fractured void space.

III. PARTICLE TREATMENT FOR VOID OR MULTI-MATERIAL CELL

For each cell, we compute the location, type, and mass for each particle in the following steps:

1. If a cell requires particle treatment or if the cell just spalled, then we move to the next step.
2. If the particles are defined previously, then the information is obtained from the particle flag word. If no particle exists, then particles will be created for each material including void.
3. Moving the particles (multi-material and material-void mixed cell) using the interpolated velocities.
4. If a mixed cell has a vacuum interface, then particles are used for the material region and no particle is assigned to the vacuum region.
5. If a void is connected to a vacuum region, then the void region is treated as a vacuum region.
6. After the particle has been moved, we save the information of the new location and the mass for each particle.
7. Ready for the next time cycle calculation.

The PIC method is well known for its expensive CPU cost and its horrendous storage requirement. We vectorized the whole code so that it would run four times faster compared to a scalar one. We saved a large amount of storage by using three packed words which will be described below. Since we were using the CRAY-XMP machine which contains 64 Bits for each word, we divided one word into many groups so that each group possessed its own information. The structure of the material flag word, MFLAG(IJ), the particle flag word, PFLAG(IJ), and the individual particle information word, PINDX(NP) are shown in Fig. 3.

Bit Structure For The Packed Array :

MFLAG (IJ)

Bits	3	18	4	8	1	2	5	5	5	5	5	3
Name		INDUV		ISM	IAPL	IFULL		MF4	MF3	MF2	MF1	MF0

PFLAG (IJ)

Bits	23	21	20
Name	INDP		INDMD

PINDX (NP)

Bits	5	19	19	21
Name	IBT	IBX	IBY	IBM

Fig. 3. Structure for the packed array MFLAG, PFLAG, and PINDX.

Definitions:

IJ: Cell at I (r-direction) and J (z-direction).

NP: Total Number of particle in cell IJ.

INDUV: Index of the velocity array, e.g., U(INDUV).

ISM: Flag to indicate spallation and melting for each material (up to maximum of 4).

IAPL: For applied pressure boundary, IAPL=1.

IFULL: 0 for empty cell, 1 for partial filled cell, 2 for full cell.

MF4-MF1: Material number index.

MFO: The total number of material in the cell.

INDP: Pointer for the particle array.

INDMD: Index for the total (summation of all particles) mass, volume, pressure, and internal energy for the first material in cell IJ.

IBT: Material type for the particle. (e.g., 1 through 31).

IBX: Normalized particle location (r-direction) in the cell (Integer < 2^{19}).

IBY: Normalized particle location (z-direction) in the cell (Integer < 2^{19}).

IBM: Normalized particle mass fraction for one type material (Integer < 2^{21}).

Where IBX is computed from the following (See Fig. 4):

$$IO = 2^{19}$$

$$DO 10 IX = 1, 8$$

$$IO = IO - 2^{16}$$

$$INXT = 28 + 8 \cdot \text{Random (between 0.0 and 1.0) (function of IX)}.$$

$$DO 10 JY = 1, 8$$

$IBX(JY) = IO + 2^{13} \cdot \text{Random}(\text{between } 0 \text{ and } 7) (\text{function of } JY) + 2^{13} \cdot \text{Random}(\text{between } 0 \text{ and } 1.0)$

10 continue.

A similar method is used to obtain the value of IBY. Where IBM is defined by:

$$IBM = \frac{\text{particle mass}}{\text{Total mass of the same material in the cell}} \times 2^{21}.$$

Fig. 4. The reference point A of any cell IJ is defined at the right-top corner with IBX, IBY indicating the position of the particle (Note: IBX and IBY are always positive).

IV. CALCULATIONS OF COPPER ROD PENETRATING STEEL PLATE

In order to check the current code capability for treating the void opening, we chose a copper rod (diameter=2cm, length=27cm and velocity = 5Km/Sec) penetrating a motionless steel disk of 5cm thick and 30cm in diameter. The initial condition and setup are given in Fig. 5. The equation of state and the formulation of the constitutive relation for shear modulus and yield strength are given in Ref. (1) which also lists the necessary parameter for copper.

For steel, the coefficients for equation-of-state in quadratic form are: $A_1 = 4.9578323$; $A_2 = 3.6883726$; $B_0 = 7.4727361$; $B_1 = 11.519148$; $B_2 = 5.5251138$; $C_0 = 0.39492613$; $C_1 = 0.52883412$; and $D_0 = 3.6$. The parameters of constitutive relation for steel are: $G_0 = 0.477$; $Y_0 = 0.0012$; $\beta = 36$; $n = 0.45$; $Y_{max} = 0.0064$; $b = 3.1446541$; $h = -0.000377358$; $q = 1.0$; $f = 0.001$; $g = 0.001$; $R' = 0.00001164$; $T_{mo} = 1790$; $\gamma_0 - a = 0.52$; $a = 1.5$; $\alpha_0 = 0.68642$; $\alpha_1 = -0.0086827$; $\alpha_2 = 0.26429125$; $\alpha_3 = 0.0068119572$; $\beta_0 = 1.0$; $\beta_1 = 0.0903$; $\beta_2 = 0.17090219$; and $\beta_3 = 0.04176577$.

The initial problem setup for the present PIC code has a window of 15 cm $\times$ 40 cm ($r \times z$) with zones of 75 $\times$ 200 (uniform grid size of 2mm). Figure 6 shows the shape of the projectile and the target at time 21 μ sec and 41 μ sec. At time 21 μ sec, the rugged surfaces on both upper and lower sides of the steel plate indicate that the spallation occurred near the surface area. This phenomena is more pronounced with the particle distributions at time 41 μ sec. The copper rod has penetrated through the steel plate at time 61 μ sec (see Fig. 7) with some perforated residue of steel. The code calculations stopped at time 71 μ sec because the rod had punched through the plate. The length of the copper rod is only 15.26 cm with 11.74 cm eroded. There are some branches at the upper part of the rod indicating that the rarefaction waves have produced spallation.

Fig. 5. The initial conditions for the copper rod and the steel plate.

Fig. 6. The shapes of the penetrator and the target at times 21 μsec and 41 μsec .

Fig. 7. The shapes of the penetrator and the target
at times 61 μsec and 71 μsec .

V. CONCLUSIONS

A particle in cell model based on the conservation of mass, momentum, and energy has been developed to solve the multi-material and void opening problems. The void growth due to fracture propagation or recombination due to compression can be described with void particle through its own velocity and volume (particle has no mass, energy, pressure, or stress). For a two-dimensional Eulerian code, the difficulty in computing the void opening resulted from material failure has been known for sometime. The present method using different types of particle to represent void or material for void-material or material-material interfacial regions. A second order accuracy is obtained for the interface tracking since we use a flux corrected transport scheme for the particle advection calculation.

Some of the programming techniques such as packing and unpacking several information word into or from one single word and the normalization of the cell-related quantities are very useful. This method coupled with the vectorization of the whole code improves the computation speed as well as the storage allocation tremendously.

REFERENCES

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