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LA-UR -87-2958

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LA-UR--87-2958

DE88 000511

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SUBMITTED TO: Published Proceedings of the Los Alamos National Laboratory Workshop on "Particle Methods in Fluid Dynamics and Plasma Physics," held April 13-15, 1987

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A GENERAL TOPOLOGY, GODUNOV METHOD

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ABSTRACT

A numerical technique that utilizes a general topology mesh is described. The method employs the arbitrary Lagrangian-Eulerian procedure and explicit, finite-volume, Godunov numerics. Material interfaces are resolved to eliminate fictitious mixing and nonphysical shear impedance. Cell-centered variables, including velocity, are used to provide consistent control volumes for the advection of mass, momentum, and energy, and to allow arbitrary slip between material regions.

The computational mesh is composed of arbitrary polygonal cells. The constraint of a fixed logical connectivity for the mesh is removed. Consequently, geometrical mesh limitations, which are responsible for inaccuracies and code failure during the evolution of region boundaries, are absent. Arbitrary boundaries can be resolved, and the mesh is capable of changing smoothly and rapidly from regions of high to low resolution. Lack of a coherent mesh orientation minimizes numerical anisotropy. A mesh rezoning approach, based on a dual triangulation and coupled with a global remapping algorithm, allows the mesh to evolve dynamically.

1. INTRODUCTION

Historically, the investigations of materials experiencing large deformations have used either an Eulerian or a Lagrangian description of the material motion. Eulerian methods are robust and well suited to model the evolution of irregular surfaces, the creation of fragments, and the description of phase changes, for example. However, the

continual remapping or advection of material properties, that is characteristic of an Eulerian description, is inherently inaccurate. Concern for accuracy is augmented when multiple materials are allowed to coexist within a computational cell. Because large changes in physical properties and discontinuities of dynamic variables are characteristic of material interfaces, their description in a mixed cell context requires either an interface reconstruction or tracking scheme. Excessive numerical diffusion, additional complication, and computational expense are incurred using this approach.

A purely Lagrangian formulation is computationally expeditious and accurate. However, Lagrangian methods are fragile. Problems involving large material deformations produce excessively distorted computational meshes, resulting in the failure of the numerical algorithm. This difficulty is mitigated by applying a Lagrangian formulation to the interfaces but allowing relative motion between the material and the computational mesh on the interior. However, if the computational mesh is constructed with logically fixed--connectivity cells, the evolution of the mesh topology is prescribed by the motion of the boundaries. Consequently, the evolution of regions of large boundary curvature may produce cells with large aspect ratios or small characteristic dimensions, which are inaccurate and impose severe time step constraints.

The utilization of arbitrary polygonal cells that lack logical connectivity is explored for solutions to material deformation problems. This approach offers the ability to resolve irregular computional regions accurately and dynamically. A two-dimensional method using a finite-volume, Godunov approach is described. The method, CAVEAT-GT, is a general topology extension to the fixed-connectivity computer code CAVEAT [1].

2. MESH GEOMETRY

The computational domain modeled by the CAVEAT-GT algorithm is divided into nonoverlapping, closed regions. Each region, typically, is associated with a specific material. Boundaries along which regions interact are referred to as interfaces. Associated

with each region is an underlying triangulation, which is used to construct the computational cells, define the mesh topology (connectivity), and describe the associated data structure. The computational cells define the control volumes used by the finite-volume formulation of the governing equations. It is from these nonoverlapping, closed, arbitrarily shaped, polygonal cells that CAVEAT-GT derives its flexibility Interior computational cells are defined by vertices that are the centroids of the underlying triangles (cf., Fig. 1). Therefore, there is a cell associated with each triangle vertex. Cells lying adjacent to boundaries also are defined by cell vertices interior to a region. Along the boundary, however, a point lying half way between the cell points is used to define the extent of the boundary cell. Such points are referred to as oundary points (cf., Fig. 1). Boundaries are constructed with linear segments defined by the cell points lying on the boundaries. Boundary segments and points that lie on the interfaces separating regions are doubly defined.

In general, calculational quantities are associated with one of three locations on a computational cell. Primary-extensive as well as the primary-intensive properties derived from them, are associated with the cell centroids. The solution of the Riemann problem and remapping also require intensive quantities on cell sides. Finally, cell vertex positions are stored.

"Fixed points" are defined as special boundary cell-points. Boundary cell-points located where three regions adjoin are referred to as triple points. The intersection of a line of symmetry and a region boundary or two lines of symmetry are fixed symmetry points. Finally, kinks or corners in the boundary contour may be defined as "fixed points" by the user. During the computation, special consideration is provided to the "fixed points" along the boundary to ensure that the interface construction algorithm does not smooth the contour in their vicinity. The locations of "fixed points" are determined prior to and remain fixed during the interface construction.

3. METHODOLOGY

CAVEAT-GT is a two-dimensional computer program written for either Cartesian or cylindrical geometries. An arbitrary Lagrangian-Eulerian (ALE) formulation is used to advance the material state one full cycle. During the Lagrangian step, the material state is advanced by obtaining solutions to the conservation equations applied to volumes following the material motion. Boundary and interface positions also are updated during this phase. Following the Lagrangian phase, a new mesh is generated. This step is the rezoning phase. Finally, in the remapping step, the variables calculated in the Lagrangian phase are transferred from their Lagrangian positions to the new mesh. In CAVEAT-GT, there are two possible rezone/remap algorithms. They include an efficient "near-Lagrangian" and a general global method. The global algorithms use the results of the "near Lagrangian" methods as their starting values. Details of the three phases are provided herein.

3.1. Lagrangian Phase

During the Lagrangian phase of the computation, the rates of change of volume, mass, momentum, and energy are updated for computational volumes following the material motion. In the finite-volume context, the equations of volume, mass, momentum, and total energy change are written

$$\frac{d}{dt}\int_{V_l} dV = \oint_{S_l} \mathbf{u}^* \cdot \mathbf{n}\, dS ,$$

$$\frac{d}{dt}\int_{V_l} \rho\, dV = 0 , \tag{1}$$

$$\frac{d}{dt}\int_{V_l} \rho \mathbf{u}\, dV = -\oint_{S_l} P^* \mathbf{n}\, dS ,$$

and

$$\frac{d}{dt}\int_{V_L} \rho E \, dV = -\oint_{S_L} P^* \mathbf{u}^* \cdot \mathbf{n} \, dS$$

An equation of state is required to close this system of equations. $V_L(t)$ is a Lagrangian control volume (i.e., a computational cell) with the surface $S_L(t)$ and moving at the local material velocity. The unit normal vector directed outward from the surface is **n**. The operator d/dt is the Lagrangian (material) time derivative. The quantities ρ, e, P, and **u** are the density, specific internal energy, pressure, and material velocity, respectively. The specific total energy is $E = e + \frac{1}{2}\mathbf{u}\cdot\mathbf{u}$. An asterisk is used to denote a cell-sided quantity.

Variables that specify the material state are stored at the centroids of the computational cells. This allows modeling gross material slip without the need to include a logical slideline. The accuracy of the method depends on the assumed spatial variation of a representative intensive quantity $\phi(\mathbf{x})$ about the cell centroid $\mathbf{x}_k$

$$\phi(\mathbf{x}) = \phi(\mathbf{x}_k) + \nabla_k\phi \cdot (\mathbf{x} - \mathbf{x}_k) + o(\Delta x^2) \tag{2}$$

The computational procedure is considered "first-order" if all quantities are assumed constant within a computational cell, that is, $\phi(\mathbf{x}) = \phi(\mathbf{x}_k)$. The method is considered "second-order" if the gradient $\nabla_k\phi$ exists, that is, a linear variation for the variable is assumed within a cell. The calculation of the cell centered gradients ($\nabla_k\phi$) includes limiting to preserve monotonicity [1].

Evaluation of the right-hand sides of Eq. (1) requires the pressure (P^*) and the normal velocity ($w^* = \mathbf{u}^* \cdot \mathbf{n}$) on the control surface. An extension of the Godunov meth

od, which solves a local Riemann problem at the cell surface, is used. The left and right states required by the Riemann solver are obtained from the cell-centroid quantities using Eq. (2). An approximate Riemann solver [3] is used in CAVEAT-GT.

Solutions to the Riemann problem provide normal material velocities, $\mathbf{w}^* = (\mathbf{u}^* \cdot \mathbf{n})\mathbf{n}$, on the cell sides. There is one Riemann velocity on each interior side and two associated with the straight line segments located along the region boundaries. These velocities are positioned mid-way between the cell point and the boundary point. Consequently, a linear distribution of the normal velocity is implied for each boundary segment. The two boundary-segment velocities are used to construct wavefronts with radius $\mathbf{w}^*\Delta t$, according to Huygens construction. The new boundary-segment position is specified by the points that lie on the tangent to the two wavefronts.

The Huygens construction is used to advance the two boundary segments that intersect at a "fixed point". The new "fixed point" position is the intersection of the advanced positions of the neighboring segments. The construction results in three potential positions for triple points. This ambiguity is resolved by linearly combining the three positions using a density weighting.

Similarly, the new boundary-cell points could be determined by the intersections of the new boundary segments. These intersections are not defined, however, when the segments are parallel or collinear. The solution to this dilemma is facilitated if the problem is posed in a variational form

$$I(\mathbf{x}_k) = \sum_k \omega_k (d^2_{m,k} + d^2_{m+1,k}) + \varepsilon \sum_m \omega_m |\mathbf{x}_{k+1} - \mathbf{x}_k|^2 , \tag{3}$$

where the sums are taken over boundary-cell points and sides, respectively. In Eq. (3), $d_{m,k}$ is the distance from the boundary points ($\mathbf{x}_k$) to the line segment m. The first term defines a variational problem for the intersection of two boundary segments. A varia

tional formulation including only this term is singuiar for parallel or collinear boundary segments. Consequently, the second term in Eq. (3) is included to regularize the variational problem. The function ω_k is chosen to decrease the contribution of the first functional as the boundary segments approach parallelism. The weight ω_m is constructed to equidistribute a "one-dimensional" mass distribution along parallel or collinear boundaries. The variation of this functional provides a system of equations for the cell-point positions ($\mathbf{x}_k$).

3.2. Rezone Phase

During the rezoning phase of the CAVEAT-GT algorithm, the location of the new mesh is determined. The positions of the boundary-cell points are determined first. Then, the boundary point locations are used as boundary conditions for the algorithm that provides the positions of the interior vertices. Both a "near-Lagrangian" and a global rezone method are available for determining the boundary and interior locations.

Advancement of the interfaces and boundaries that enclose each region is accomplished by the interface construction technique (cf., Sec. 3.1). This construction uses the velocities normal to the boundary segments to position the new boundary. Location of the boundary-cell points tangentially along the boundary segments is arbitrary. Placement of the boundary points along the segments that are obtained from the interface construction is performed by the boundary rezone algorithm. The "near-Lagrangian" placement locates the boundary points to preserve the original mass distribution along the boundary segments. The associated advection across cell sides that intersect the boundary is minimized.

The general topology mesh offers the ability to add computational cells in regions demanding finer resolution and eliminating cells where they no longer are required along the boundary. This is accomplished by calculating a point distribution parameter N from the ordinary differential equation

$$\frac{dN}{dS} = f(s, \kappa, \nabla\phi, \ldots) \; . \tag{4}$$

The point-distribution density function (f) is chosen to distribute boundary points equally along the interfaces in the absence of any distinguishing features. Otherwise, boundary points are forced to migrate into regions with large values of the boundary curvature (κ) or the gradient ($\nabla\phi$) of a prescribed variable, such as pressure. Equation (4) is integrated along boundary contours between "fixed points." The resulting values for N(s) are scaled to ensure that the final value for N(s = L) is an integer. That is, the positions of the "fixed points" are not altered. The boundary points then are placed along the boundary contour at positions where N(s) has integer values. Solutions for N(s) are obtained every time-step. The solution is tested to determine if the existing boundary-point distribution sufficiently resolves the boundary contour. If boundary point addition or deletion or gross vertex migration is unnecessary, the boundary-point positions resulting from the "near-Lagrangian" description are used. However, if the "near-Lagrangian" positions are not adequate to resolve accurately the boundary contour, then the final positions of the boundary points are specified by Eq. (4) and a global rezone of the interior mesh also is required.

The interior rezone algorithms construct a mesh on the interior of each region. The interior mesh construction schemes require the boundary-point positions, obtained from the boundary rezone computation, as boundary conditions. Both of the interior-rezone algorithms manipulate the triangulation, rather than the computational mesh. If the Lagrangian cell vertex positions were available, remapping the variables obtained from the Lagrangian phase of the calculation would be unnecessary. Unfortunately, it is possible to collapse small cell sides without substantially affecting the cell volume with a purely Lagrangian description. The "near-Lagrangian" rezone approach attempts to preserve the cell volumes produced by the material motion and maintain a smooth mesh.

The "near-Lagrangian" mesh velocities (u_m) are obtained from the solution to the equation

$$\nabla^2 u_m \equiv 1/v\, dv/dt \,, \tag{5}$$

where v is the specific Lagrangian volume. This formulation preserves Lagrangian volumes.

If the computational mesh becomes sufficiently distorted, then a global-rezone method is employed to produce a smooth mesh. A global rezone is invoked if solutions to Eq. (5) produce triangles with negative areas or if an interior triangle contains an angle less than 10 degrees. A global rezone also is performed when points are added or deleted along the boundary, or there is gross boundary point migration. Similar to established rezoning techniques [4], a variational formulation using a composite functional, which will produce desirable mesh characteristics, is used. The functional incorporated into the CAVEAT-GT method is

$$I = \sum_n (d_{12}^2 + d_{23}^2 + d_{31}^2)_n / A_n + \alpha \sum_m d_m^2 \,, \tag{6}$$

where the sums are taken over traingles and cell sides, respectively. The first term in Eq. (C) provides a measure of the smoothness of the computational mesh. A_n is the triangle area and d_{ij} is the length of the triangle side. A variational formulation composed only of this first term attempts to produce equilateral triangles. However, the triangle areas could be grossly disparate. The second term in Eq. (6) is included to mitigate this difficulty. This functional is minimized when the lengths of the triangle sides (d_m) are equal. Changes in the connectivity of the mesh are allowed during the iterative procedure used to minimize Eq. (6). Point addition or deletion on the mesh interior is precluded.

3.3. Remap Phase

Although the normal motion of the region boundaries is Lagrangian, the mesh motion tangent to the boundaries and on the interior differ from the material motion. Consequently, it is necessary to remap the results of the Lagrangian phase onto the mesh positions dictated by the rezoning algorithms. Remapping procedures introduce a diffusion error into the results. This error is reduced by increasing the order of accuracy of the approach or reducing the relative difference between the material and mesh velocities.

If the difference between the material and mesh velocities is sufficiently small to preclude violating the stability of the numerical technique, then the variables may be advected to the new mesh. Advection, therefore, is appropriate when remapping to the mesh generated by the "near-Lagrangian" rezoning technique. In the event that an entirely new mesh is generated, a global remap of the material variables is required. Because the variables are remapped from the "near-Lagrangian" positions to the new mesh, a global rezone/remap always is preceded by a "near-Lagrangian" rezone and advection. The global remap contained in CAVEAT-GT is an extension of previously developed methods for quadrilaterals [5]-[8] to the geometry of a general topology mesh. A conservative transfer of the variables between two meshes is obtained. There is no restriction on either the mesh topology or the time-step size.

4. EXAMPLE PROBLEMS

Two test problems are presented to demonstrate the features of the general topology formulation. A dimensionless set of units is used in the problem descriptions.

4.1. Blast Wave

The blast wave problem is composed of one region with seven fixed boundaries (i.e., reflective boundary conditions) and 593 computational cells. The characteristic cell dimension is approximately 0.08. Initially, the velocity, pressure, density, and specific internal energy are 0, 1×10^{10}, 1, and 1.5×10^{10}, respectively. At $t = 0$, a source of

energy is applied to the cell located at x = y = 0.95. This computational cell is assigned the values of 20/3, 1, and 10 for the pressure, density, and specific internal energy, respectively. A gamma-law gas equation-of-state with $\gamma = 5/3$ is used.

As the calculation evolves, a wave emanates from the energy source. The "near-Lagrangian" rezone algorithm concentrates cells in the vicinity of the wave. As cells are compressed in the neighborhood of the wave, distorted triangles are generated. When this occurs, a global rezone is performed and a more regular mesh is generated. Mesh geometries preceding and following a global rezone are provided in Fig. 2. It is observed, that although a smoother mesh is produced, a region of smaller cells remains in the vicinity of the wave. Pressure profiles preceding and following a global remap also are provided in Fig. 3 for a first-order calculation. The diffusion produced by the remapping is evident.

4.2. Impact Problem

Consider a thin plate with dimensions 0.4 by 2.0, density of 8.9, and traveling at the uniform velocity of -0.196 in the vertical direction. At t = 0 the plate encounters a rigid wall. The impact problem is modeled using the general topology method and a fixed-connectivity mesh with the identical Godunov numerics for comparison. Both meshes use computational cells with a characteristic dimension of 0.1. The left and bottom boundaries are reflective. The right and top boundaries are a free surface (P = 0) and a specified velocity boundary (v = -0.196), respectively. A Chaplygin equation-of-state is used

$$P = k^2\left(\frac{1}{\rho_0} - \frac{1}{\rho}\right), \tag{7}$$

where k = 3.49 and ρ_0 = 8.9.

The mesh evolution for a second-order, van Leer limited calculation using the general-topology mesh is shown in Fig. 4. The ability of the technique to smoothly add and delete computational cells along the boundaries is evident. For comparison, the late time mesh for a second-order, van Leer limited, fixed-connectivity computation also is provided in Fig. 5. The fixed-connectivity calculation also utilized a mesh rezoning technique in an effort to maintain a regular mesh in the interior. The accuracy of this latter calculation is suspect at later times as cell aspect ratios become excessive. Both calculations are explicit. Consequently, as the characteristic dimension of the mesh decreases for the fixed-connectivity analysis, the time-step size decreases. At t = 7.5, the time-step sizes are 2.4×10^{-2} and 3.8×10^{-3} for the general-topology and fixed-connectivity methods, respectively.

A steady-state, analytic solution is available for the impact problem [9]. To simulate steady-state conditions, late time solutions for a plate with a width-to-height ratio of 0.5:7.5 are obtained. Initially, the plate is in uniform motion with values of -1. and 1. for the vertical velocity and density, respectively. The left and bottom boundaries are reflective. The right boundary is a free surface and the top boundary is a specified velocity boundary with v = -1.0. The initial mesh is composed of 512 computational cells with a characteristic dimension of 0.1. A Chaplygin equation-of-state [cf., Eq. (7)] is used with k = 3.49 and ρ_0 = 1.0.The results for a late time, second-order, van Leer limited calculation is provided in Fig. 6.

5. CONCLUSIONS

A two-dimensional, general-topology, Godunov method has been developed. The use of general polygonal cells facilitates the dynamic resolution of problems involving large material deformations. The formulation uses a Lagrangian description for material boundaries. Consequently, an accurate boundary analysis that eliminates fictitious shear impedance and intermaterial penetration results.

Future extensions of the numerical method are envisioned. The ability to add or delete computational cells on the interior and the inclusion of a more general set of boundary conditions is planned. Finally, because the existing code is used for an experimental investigation, no attempt has been made to develop a fast version, although optimizing and vectorizing of the coding is possible.

REFERENCES

[1] F. L. Addessio, D. E. Carroll, J. K. Dukowicz, F. H. Harlow, J. N. Johnson, B. A. Kashiwa, M. E. Maltrud, and H. M. Ruppel, "CAVEAT: A Computer Code for Fluid Dynamic Problems with Large Distortion and Internal Slip," Los Alamos National Laboratory report LA-10613-MS (1986).

[2] B. van Leer, "Towards the Ultimate Conservative Difference Scheme. V. A Second-Order Sequel to Godunov's Method," *J. Compt. Phys.* **32**, 101-136 (1979).

[3] J. K. Dukowicz, "A General Non-Iterative Riemann Solver for Godunov's Method," *J. Comp. Phys.* **61**, 119-137 (1985).

[4] J. U. Brackbill and J. S. Saltzman, "Adoptive Zoning for Singular Problems in Two Dimensions," *J. Compt. Phys.* **46**, 342-368 (1982).

[5] J. K. Dukowicz, "Conservative Rezoning (Remapping) for General Quadrilateral Meshes, *J. Comp. Phys.* **54**, 411-424 (1983).

[6] J. D. Ramshaw, "Conservative Rezoning Algorithm for Generalized Two-Dimensional Meshes," *J. Comp. Phys.* **59**, 193-199 (1985).

[7] J. D. Ramshaw, "Simplified Second-Order Rezoning Algorithm for Generalized Two-Dimensional Meshes," *J. Comp. Phys.* **67**, 214-221 (1986).

[8] J. K. Dukowicz and J. W. Kodis, "Accurate Conservative Remapping (Rezoning) for Arbitary Lagrangian-Eulerian Computations," *SIAM J. Sci. Stat. Comp.* (in press).

[9] R. R. Karp, "An Exact Partial Solution to the Steady-State, Compressible Fluid Flow Problems of Jet Formation and Jet Penetration," Los Alamos Scientific Laboratory report LA-8371 (1980).

FIGURE CAPTIONS

Fig. 1. Mesh Geometry (--- triangulation, — cell, o cell point, □ cell vertex, ▲ boundary point).

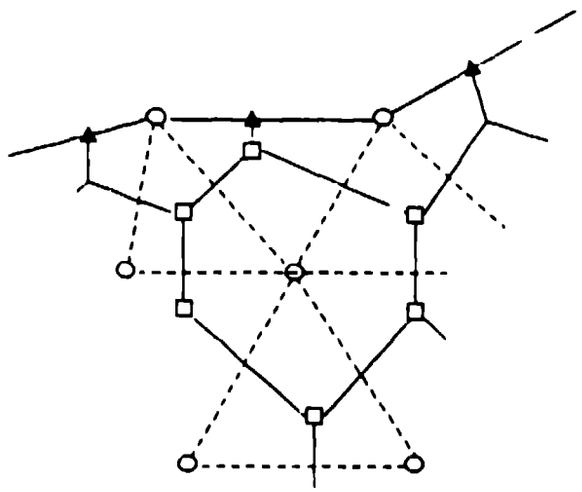
Fig. 2. Mesh Geometry (a) Preceding and (b) Following a Global Rezone for the Blast Wave Problem.

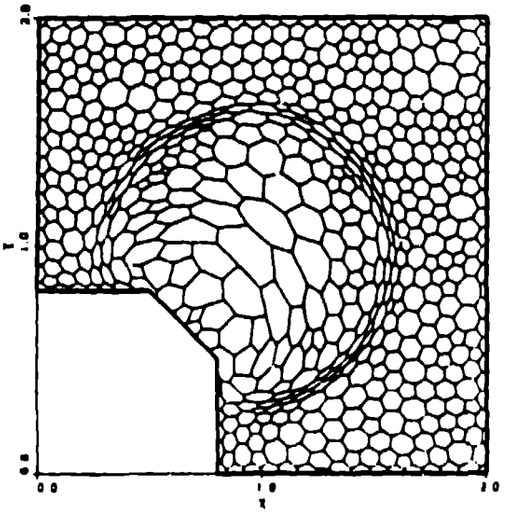
Fig. 3. Pressure Profiles (a) Preceding and (b) Following a Global Rezone for the Blast Wave Problem.

Fig. 4. Mesh Evolution of the Impact Problem for the General Topology Method at (a) $t = 2.0$ and (b) $t = 7.5$.

Fig. 5. Mesh Geometry of the Impact Problem for the Fixed-Connectivity Method at $t = 7.5$.

Fig. 6. Comparison of the (a) Density and (b) Velocity for the Steady-State, Impact Problem along the Impact Plane (-- analytic and o computational result).





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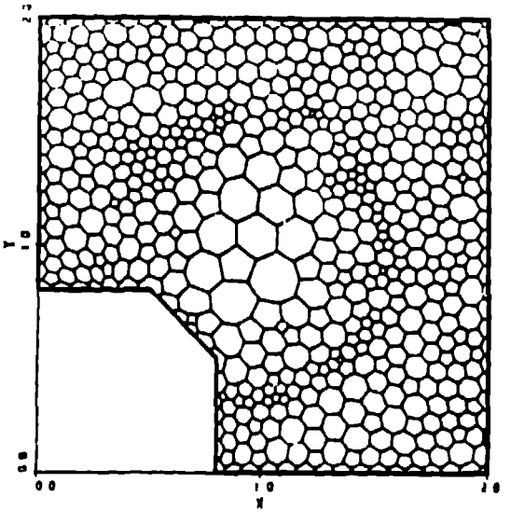

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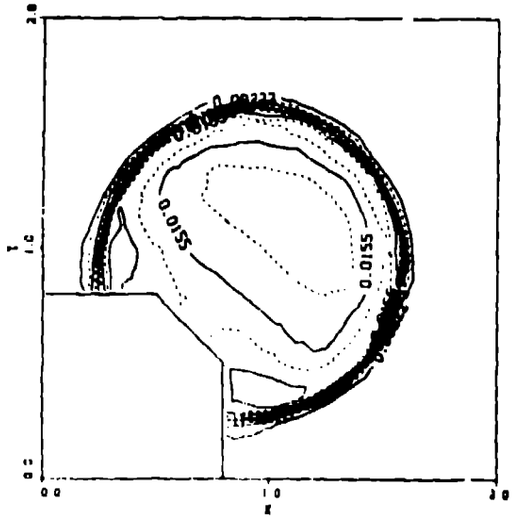

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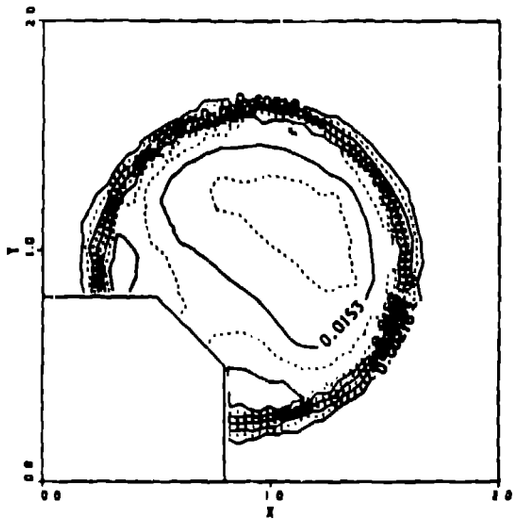

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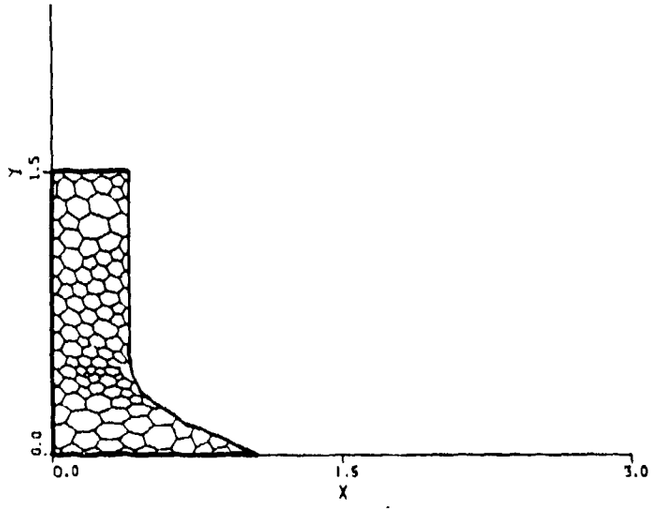

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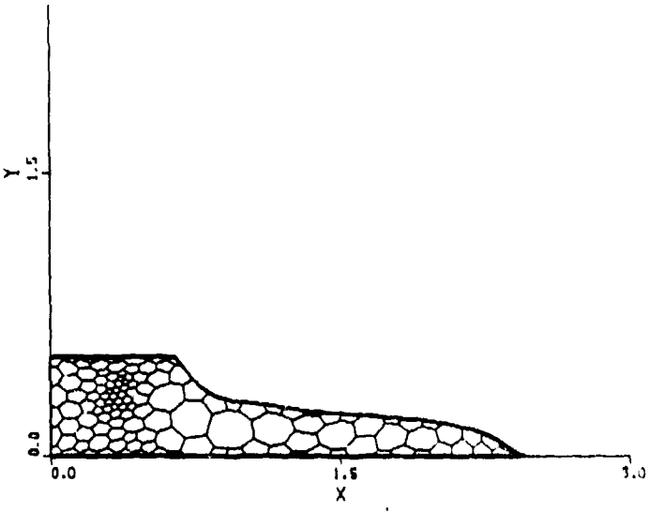

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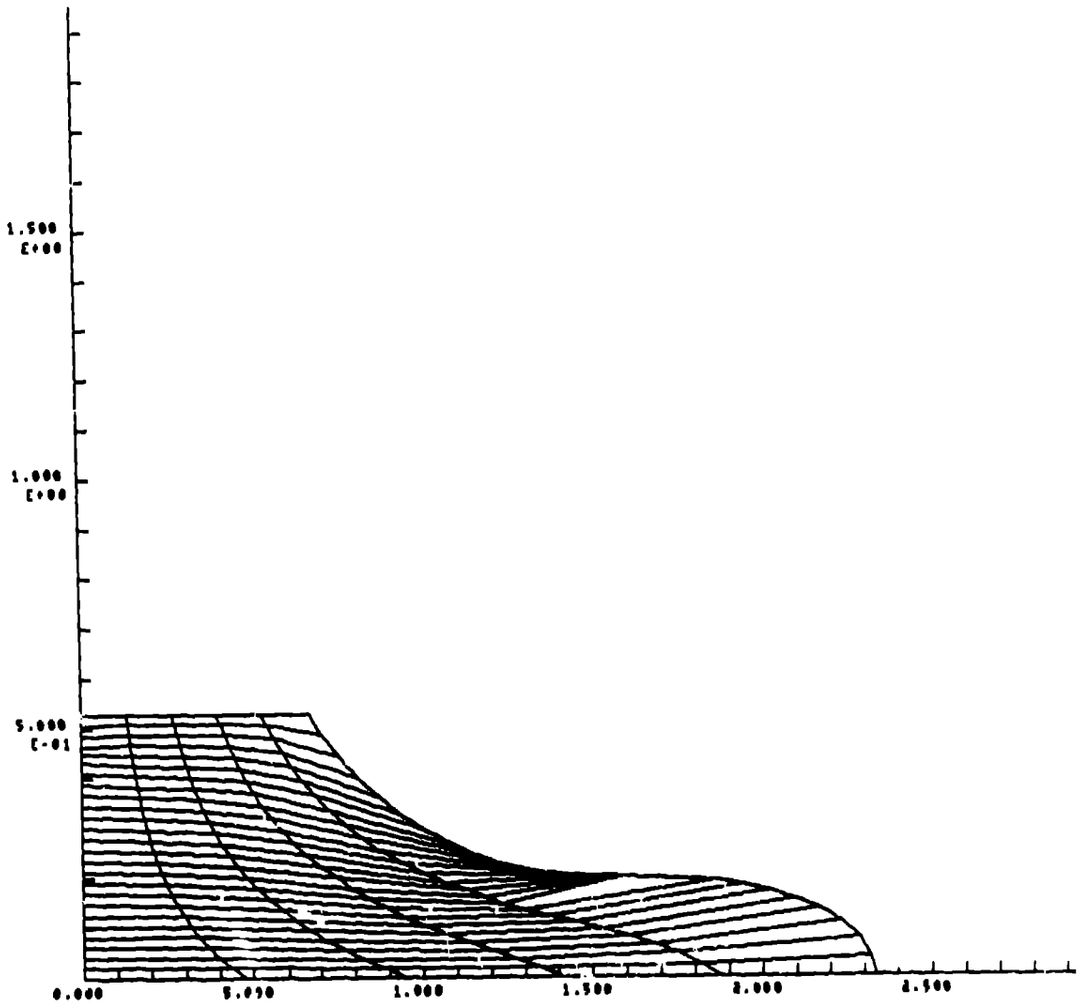
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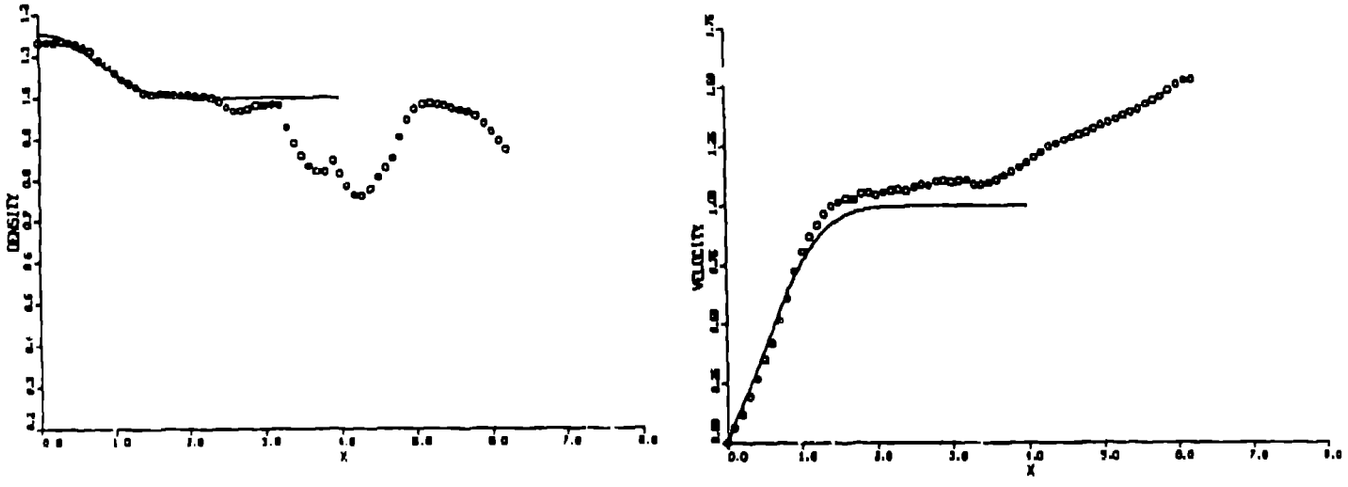

(a) (b)