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Compatible, Energy and Symmetry Preserving 2D Lagrangian Hydrodynamics in rz - Cylindrical Coordinates

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We present a new discretization for 2D Lagrangian hydrodynamics in rz geometry (cylindrical coordinates) that is compatible, energy conserving and symmetry preserving. We describe discretization of the basic Lagrangian hydrodynamics equations. This formulation can be used for general polygonal meshes, however in this paper we only describe it for logically rectangular grid. We show that our discretization preserves spherical symmetry on polar equiangular meshes. The discretization conserves total energy exactly up to machine roundoff on any mesh. It has a consistent definition of kinetic energy in the zone that is exact for a constant velocity field.

The method is based on ideas presented in [1, 2], where the authors use a special procedure to distribute zonal mass to corners of the zone (subzonal masses). The momentum equation is discretized in its "Cartesian" form with a special definition of "planar" masses (area-weighted).

Two principal contributions of this paper are as follows: first is a definition of "planar" subzonal mass for nodes on the z axis ($r = 0$) that does not require a special procedure for movement of these nodes. Second is proof that the discretization preserves spherical symmetry including analysis internal energy equation.

We present numerical examples that demonstrate the robustness of the new method.

1. GAS DYNAMICS EQUATIONS IN AXISYMMETRIC GEOMETRY

Momentum Equation. General form of momentum equation for Lagrangian parcel $V(t)$ is

$$\frac{d}{dt} \left(\int_{V(t)} \mathbf{u} \rho dV \right) = - \oint_{\partial V(t)} p \mathbf{n} dS. \quad (1)$$

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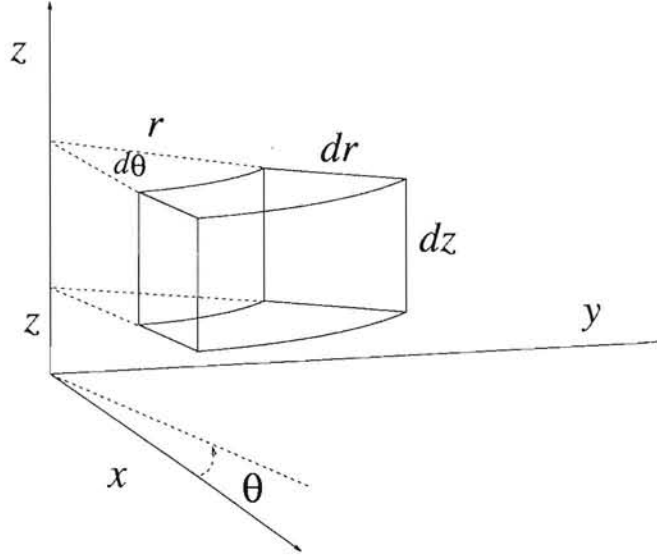


Figure 1. Control volume

One can obtain the following conservative form of momentum equation in $r - z$ axisymmetric geometry

$$r \rho \frac{du}{dt} = - \left(\frac{\partial(r p)}{\partial r} - p \right), \quad r \rho \frac{dv}{dt} = - \frac{\partial(r p)}{\partial z} \quad (2)$$

if general formula (1) is applied to control volume presented in Fig. 1, here u and v are in r and z components of the velocity vector correspondingly.

Equation for specific internal energy, ε has the following form

$$r \rho \frac{d\varepsilon}{dt} = -p \left(\frac{\partial(r u)}{\partial r} + \frac{\partial(r v)}{\partial z} \right). \quad (3)$$

To compute complex flows with shocks it is very important to conserve total energy, which is defined as follows Specific total energy, E , for axisymmetric flow is

$$E = \int_{V(t)} \left(\varepsilon + \frac{u^2 + v^2}{2} \right) \rho dV. \quad (4)$$

General form of conservation of total energy is

$$\frac{d}{dt} \left(\int_{V(t)} E \rho dV \right) = - \oint_{\partial V(t)} p \mathbf{u} \cdot \mathbf{n} dS. \quad (5)$$

If initial and boundary conditions specified appropriately then equations in cylindrical coordinates allow spherically symmetric solution. That is, density, internal energy

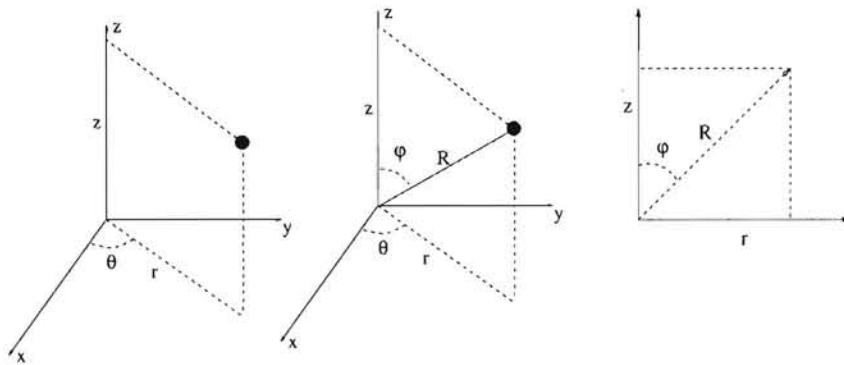


Figure 2. Cartesian - (x, y, z) , Cylindrical - $(r = \sqrt{x^2 + y^2}, z, \theta)$, and Spherical Coordinates - $(R = \sqrt{r^2 + z^2}, \theta, \varphi)$

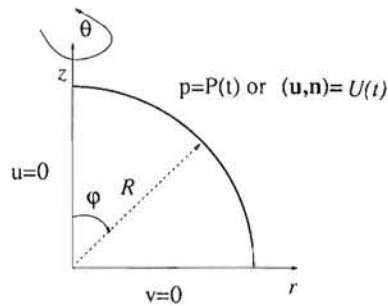


Figure 3. Boundary conditions for spherically symmetric problem

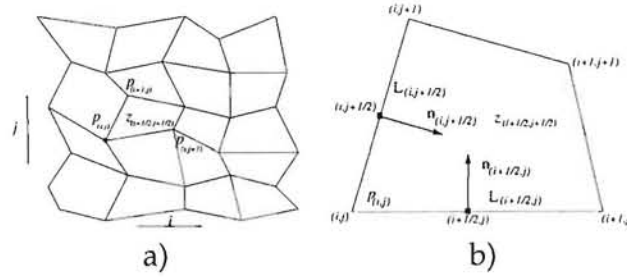


Figure 4. Logically rectangular grid: a) Entire grid, b) Zone $(i + \frac{1}{2}, j + \frac{1}{2})$ and corresponding notations

and pressure depend only of spherical radius ($R = \sqrt{r^2 + z^2}$): $\rho(r, z) = \rho(R, t)$, $\varepsilon(r, z) = \varepsilon(R, t)$, $p(r, z) = p(R)$, and velocity can be represented as follows $u = U(R) \sin \varphi$, $v = U(R) \cos \varphi$, where coordinate systems are represented in Fig. (2).

Boundary conditions for spherically symmetric problems are presented in Fig. 3.

For spherically symmetric problems acceleration $\mathbf{a} = (a_u, a_v)$ is directed in radial direction and its amplitude depends only on spherical radius R :

$$a_u = -\frac{1}{\rho(R)} \frac{\partial p(R)}{\partial R} \sin \varphi, \quad a_v = -\frac{1}{\rho(R)} \frac{\partial p(R)}{\partial R} \cos \varphi. \quad (6)$$

Equation for internal energy has the following form:

$$\frac{d\varepsilon}{dt} = -\frac{1}{\rho(R)} p(R) \cdot \left(\frac{1}{R^2} \frac{\partial(R^2 U)}{\partial R} \right), \quad (7)$$

that is $\varepsilon = \varepsilon(R, t)$.

2. COMPATIBLE STAGGERED DISCRETIZATION

For simplicity of presentation, in this paper we will consider semi-discrete discretizations, that is we will keep time continuous and consider only spatial discretization.

In this paper we consider logically rectangular grid, Fig. 4, where each point, p , can be enumerated by two integer indices (i, j) , and each zone, z , enumerated by two half indices $i + \frac{1}{2}, j + \frac{1}{2}$.

In staggered discretization point quantities are coordinates, (r_p, z_p) , and velocity components, (u_p, v_p) . Zonal quantities are volume, V_z , density, ρ_z , mass m_z , internal energy, ε_z and pressure p_z .

For Lagrangian methods: $d(m_z)/dt = 0$ $m_z = \rho_z|_{t=0} \cdot V_z|_{t=0}$. Therefore, for any time moment t density can be defined as follows $\rho_z(t) = m_z/V_z(t)$, which plays the role of discrete continuity equation. Also for Lagrangian methods each point moves with fluid velocity, that is, $d(r_p)/dt = u_p$, $d(z_p)/dt = v_p$.

Zonal internal energy is $\mathcal{E}_p = m_z \varepsilon_z$, and point momentum, μ_p , and kinetic energy,

K_p , are defined as follows

$$\mu_p = m_p \mathbf{u}_p, \quad K_p = m_p \frac{|\mathbf{u}_p|^2}{2}$$

where m_p - point mass, which has to be defined.

There are following obvious requirements for point mass.

$$d(m_p)/dt = 0; \quad \sum_z m_z = \sum_p m_p.$$

Following [1], we introduce additional Lagrangian objects, so-called, subzonal masses, m_z^p , such that $d(m_z^p)/dt = 0$ and

$$\sum_{p \in \mathcal{P}(z)} m_z^p = m_z, \quad (8)$$

where $\mathcal{P}(z)$ is set of vertices of zone z . Then point mass can be defined as follows $m_p = \sum_{z \in \mathcal{Z}(p)} m_z^p$. where $\mathcal{Z}(p)$ is set of zones which have point p as vertex.

It is important to note that if one defines subzonal volume $V_z^p(t)$ in some consistent way, such that $\sum_{p \in \mathcal{P}(z)} V_z^p(t) = V_z(t)$, then it leads to natural definition of subzonal density

$$\rho_z^p(t) = m_z^p / V_z^p(t). \quad (9)$$

Generic compatible form of discrete momentum and internal energy equations is

$$m_p \frac{d\mathbf{u}_p}{dt} = \sum_{z \in \mathcal{P}(z)} \mathbf{f}_z^p, \quad m_z \frac{d\varepsilon_z}{dt} = - \sum_{p \in \mathcal{Z}(p)} \mathbf{f}_z^p \cdot \mathbf{u}_p.$$

Therefore spatial discretization is completely defined, if we define subzonal masses m_z^p and subzonal forces \mathbf{f}_z^p . In simplest case, which we will consider in this paper, subzonal force depends on the geometry of the zone and zonal pressure.

For compatible discretizations, evolution of total kinetic energy, $K = \sum_p K_p$ is $\frac{dK}{dt} = \sum_p \left(\sum_{z \in \mathcal{P}(z)} \mathbf{f}_z^p \cdot \mathbf{u}_p \right)$, and evolution of total internal energy, $\mathcal{E} = \sum_p \mathcal{E}_p$ is $\frac{d\mathcal{E}}{dt} = - \sum_z \left(\sum_{p \in \mathcal{Z}(p)} \mathbf{f}_z^p \cdot \mathbf{u}_p \right)$. Therefore change in total energy $E = \mathcal{K} + \mathcal{E}$

$$\frac{dE}{dt} = \sum_p \left(\sum_{z \in \mathcal{P}(z)} \mathbf{f}_z^p \cdot \mathbf{u}_p \right) - \sum_z \left(\sum_{p \in \mathcal{Z}(p)} \mathbf{f}_z^p \cdot \mathbf{u}_p \right) = \text{boundary terms},$$

which is discrete form of "conservation" of total energy.

3. DEFINITION OF SUBZONAL MASSES

Discretization of momentum equation, which preserves spherical symmetry is based on non-conservative ("Cartesian") form of momentum equation

$$\rho \frac{du}{dt} = - \frac{\partial p}{\partial r}, \quad \rho \frac{dv}{dt} = - \frac{\partial p}{\partial z}, \quad (10)$$

which is equivalent to (2) in differential case.

General control volume derivation of discrete form of "Cartesian" form of momentum equation gives

$$\langle \rho A \rangle_p(t) \frac{d\mathbf{u}_p}{dt} = \sum_{z \in \mathcal{Z}(p)} (\mathbf{f}_{cart})_z^p, \quad (11)$$

where $\langle \rho A \rangle_p(t) \approx \int_{z(t)} \rho(r, z, t) dr dz$. Generic discrete form of $\langle \rho A \rangle_p(t)$ is $\langle \rho A \rangle_p(t) = \sum_{z \in \mathcal{Z}(p)} (\rho_z^p)(t) (A_z^p)(t)$, where $(\rho_z^p)(t)$ and $(A_z^p)(t)$ has to be defined. For symmetry preservation it can be any symmetric quadrature around the point. Necessary condition for zero order approximation is

$$\sum_{p \in \mathcal{P}(z)} (A_z^p)(t) = (A_z)(t). \quad (12)$$

Discrete equation (11) is not in compatible form, therefore to construct conservative discretization we need to define $(\rho_z^p)(t)$ and $(A_z^p)(t)$ in such a way that equation (11) can be rewritten in equivalent compatible form:

$$m_p \frac{d\mathbf{u}_p}{dt} = \sum_{z \in \mathcal{P}(z)} \mathbf{f}_z^p, \quad (13)$$

where m_p corresponds to true cylindrical mass - $\int_{V(t)} \rho r dr dz$. Comparison of (13) and (11) leads to following definition of m_p and \mathbf{f}_z^p

$$m_p = r_p(t) \left(\sum_{z \in \mathcal{Z}(p)} (\rho_z^p)(t) (A_z^p)(t) \right), \quad \mathbf{f}_z^p(t) = r_p(t) (\mathbf{f}_{cart})_z^p(t). \quad (14)$$

Using notion of subzonal masses we will present point point mass as follows

$$m_p = \sum_{z \in \mathcal{Z}(p)} m_z^p, \quad m_z^p = (\rho_z^p)(t) r_p(t) (A_z^p)(t) = (\rho_z^p)|_{t=0} r_p|_{t=0} (A_z^p)|_{t=0}. \quad (15)$$

It leads to natural definition of subzonal volume

$$V_z^p(t) = r_p(t) A_z^p(t). \quad (16)$$

Equation (8) leads to following requirement for A_z^p

$$\sum_{p \in \mathcal{P}(z)} (V_z^p)(t) = \sum_{p \in \mathcal{P}(z)} (r_p)(t) (A_z^p)(t) = V_z(t). \quad (17)$$

Therefore, we need to find $A_z^p(t)$ which satisfies two conditions (12),(17). One of the possible solutions for quad mesh is presented in [1]:

$$\begin{aligned} A_z^1 &= \frac{5 A_{41} + 5 A_{12} + A_{23} + A_{34}}{12}, & A_z^2 &= \frac{A_{41} + 5 A_{12} + 5 A_{23} + A_{34}}{12} \\ A_z^3 &= \frac{A_{41} + A_{12} + 5 A_{23} + 5 A_{34}}{12}, & A_z^4 &= \frac{5 A_{41} + A_{12} + A_{23} + 5 A_{34}}{12}, \end{aligned}$$

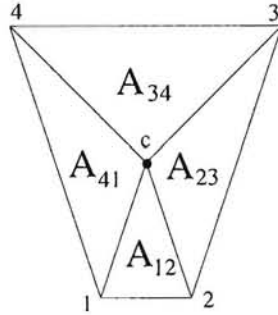


Figure 5. Volume Distribution. Geometric center of the quad is $r_c = (r_1 + r_2 + r_3 + r_4)/4$, $z_c = (z_1 + z_2 + z_3 + z_4)/4$

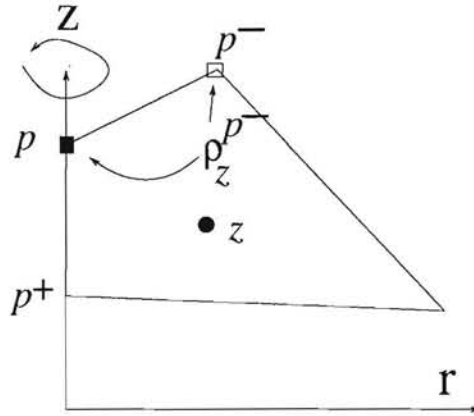


Figure 6. Definition of subzonal density for points on z axis

where corresponding triangles are presented in Fig. 5

For point which are not on z axis subzonal volume V_z^p defined by equation (16) is positive and therefore subzonal density can be defined using equation (9). However, for points on z axis $m_z^p = 0$ and $V_z^p = 0$, therefore we need to define corresponding subzonal density using some other means. It suppose to satisfy some minimal requirements of consistency and also preserve spherical symmetry on special meshes.

For logically rectangular mesh each point on z axis is connected to only one point which is not on the axis by edge of the zone. For example, in Fig. 6 for point p on z axis such point is p^+ . In this situation we set

$$\rho_z^p(t) = \rho_z^{p^+}(t). \tag{18}$$

Let us note that such definition of subzonal density does not affect corresponding subzonal mass, which is zero because corresponding subzonal volume is zero.

Now let us consider how it affects logic of the compatible discretization. First of all, if we define zonal kinetic energy as follows

$$K_z = \sum_{p \in \mathcal{P}(z)} \frac{m_z^p |\mathbf{u}_p|^2}{2} \sim \int_{V_z} \rho \frac{|\mathbf{u}_p|^2}{2} dV$$

then minimal consistency condition means that if \mathbf{u} is constant then K_z suppose to be exact, which is clearly true in our discretization because of definition of subzonal volumes.

Second, kinetic energy does not depend on velocity in points on z axis because corresponding $m_z^p = 0$. Therefore, movement of points on the boundary (which is affected by definition of corresponding subzonal masses) does not contribute to instantaneous energy balance. Third, definition of zonal internal energy does not depend on m_z^p $\mathcal{E}_z = m_z \varepsilon_z$, as long corresponding m_z^p sum to m_z , which is true in our case. Therefore logic of compatible discretization is not affected and our discretization conserves total energy.

4. DISCRETE EQUATIONS ON LOGICALLY RECTANGULAR GRID

On general logically rectangular grid discretization of "Cartesian" forces follows from definition of "Cartesian" gradient operator -

$$\int_{A(t)} \text{grad}_{\text{cart}} p dA = \oint_{\partial A(t)} p \mathbf{n} dl;$$

Using notations for points and zones for logically rectangular grid we obtain the following expression for subzonal forces

$$(\mathbf{f}_{\text{cart}})_{i+\frac{1}{2},j+\frac{1}{2}}^{i,j} = p_{i+\frac{1}{2},j+\frac{1}{2}} \left(\frac{L_{i+\frac{1}{2},j}}{2} \mathbf{n}_{i+\frac{1}{2},j} + \frac{L_{i,j+\frac{1}{2}}}{2} \mathbf{n}_{i,j+\frac{1}{2}} \right).$$

Corresponding discretization of momentum equation is

$$\begin{aligned} \langle \rho A \rangle_{i,j}^n \frac{d\mathbf{u}_{i,j}}{dt} = & \\ -\frac{1}{2} \left\{ \left[L_{i+\frac{1}{2},j} \left(p_{i+\frac{1}{2},j+\frac{1}{2}} - p_{i+\frac{1}{2},j-\frac{1}{2}} \right) \mathbf{n}_{i+\frac{1}{2},j} + L_{i-\frac{1}{2},j} \left(p_{i-\frac{1}{2},j+\frac{1}{2}} - p_{i-\frac{1}{2},j-\frac{1}{2}} \right) \mathbf{n}_{i-\frac{1}{2},j} \right] + \right. & \\ \left. \left[L_{i,j+\frac{1}{2}} \left(p_{i+\frac{1}{2},j+\frac{1}{2}} - p_{i-\frac{1}{2},j+\frac{1}{2}} \right) \mathbf{n}_{i,j+\frac{1}{2}} + L_{i,j-\frac{1}{2}} \left(p_{i+\frac{1}{2},j-\frac{1}{2}} - p_{i-\frac{1}{2},j-\frac{1}{2}} \right) \mathbf{n}_{i,j-\frac{1}{2}} \right] \right\}. & \end{aligned}$$

Equation for internal energy looks as follows

$$\begin{aligned} m_{i+\frac{1}{2},j+\frac{1}{2}} \frac{\varepsilon_{i+\frac{1}{2},j+\frac{1}{2}}^{n+1} - \varepsilon_{i+\frac{1}{2},j+\frac{1}{2}}^n}{\Delta t} = & -p_{i+\frac{1}{2},j+\frac{1}{2}} \left\{ \right. \\ \left[L_{i+\frac{1}{2},j+1} \mathbf{n}_{i+\frac{1}{2},j+1} \cdot \frac{r_{i,j+1}^n \mathbf{u}_{i,j+1} + r_{i+1,j+1}^n \mathbf{u}_{i+1,j+1}}{2} - L_{i+\frac{1}{2},j} \mathbf{n}_{i+\frac{1}{2},j} \cdot \frac{r_{i,j}^n \mathbf{u}_{i,j} + r_{i+1,j}^n \mathbf{u}_{i+1,j}}{2} \right] + & \\ \left[L_{i+1,j+\frac{1}{2}} \mathbf{n}_{i+1,j+\frac{1}{2}} \cdot \frac{r_{i+1,j}^n \mathbf{u}_{i+1,j} + r_{i+1,j+1}^n \mathbf{u}_{i+1,j+1}}{2} - L_{i,j+\frac{1}{2}} \mathbf{n}_{i,j+\frac{1}{2}} \cdot \frac{r_{i,j}^n \mathbf{u}_{i,j} + r_{i,j+1}^n \mathbf{u}_{i,j+1}}{2} \right] & \left. \right\} \end{aligned}$$

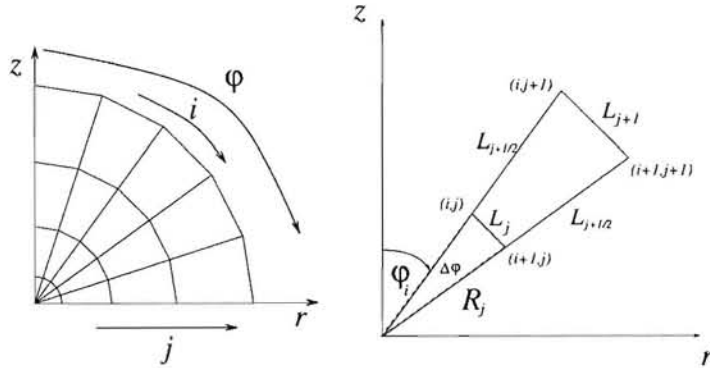


Figure 7. Equiangular polar mesh: a) Entire mesh, b) One cell

5. PRESERVATION OF SPHERICAL SYMMETRY ON EQUIANGULAR POLAR MESH

In this section we show that our new discretization preserves spherical symmetry on special equiangular polar meshes, Fig. 7 a).

Coordinates of points of such mesh are defined as follows

$$r_{i,j} = R_j \sin \varphi_i, \quad z_{i,j} = R_j \cos \varphi_i; \quad i = 1, \dots, I; j = 1, \dots, J,$$

$$\varphi_i = (i - 1) \Delta\varphi; \quad \Delta\varphi = \frac{\pi/2}{I - 1}.$$

Statement of exact preservation of spherical symmetry on polar mesh can be formulated as follows. Corresponding components of the velocity are equal to zero on axis: $u_{1,j}(t) = 0; v_{I,j}(t) = 0$. Both components of the velocity is zero at the origin $u_{1,1}(t) = v_{1,1}(t) = 0$. On outer boundary one can specify pressure as the function of the time - $p_{i+1/2,j}(t) = P_{top}(t)$, or normal component of the velocity as function of time - $u_{i,j}(t) \sin \theta_i + v_{i,j}(t) \cos \theta_i = U(t^n)$.

Initial conditions for scalar functions are as follows $\rho_{i+1/2,j+1/2}|_{t=0} = \rho_{j+1/2}|_{t=0}; p_{i+1/2,j+1/2}|_{t=0} = p_{j+1/2}|_{t=0}, \varepsilon_{i+1/2,j+1/2}|_{t=0} = \varepsilon_{j+1/2}|_{t=0}$. Initial velocity directed radially and its magnitude depends only on j : $u_{i,j}|_{t=0} = U_j|_{t=0} \cdot \sin \theta_i$ and $v_{i,j}|_{t=0} = U_j|_{t=0} \cdot \cos \theta_i$.

If for these initial and boundary conditions, the density, internal energy and pressure depend only on j and the velocity is spherical—that is, $u_{i,j}(t) = U_j(t) \sin \theta_i$ and $v_{i,j}(t) = U_j(t) \cos \theta_i$ at all later times, then we say that the finite difference scheme preserves spherical symmetry.

On polar equiangular mesh momentum equation can be written in the following form

$$\mathbf{a}_{i,j} = \frac{d\mathbf{u}_{i,j}}{dt} = \left\{ \frac{R_j \left(p_{j+\frac{1}{2}} - p_{j-\frac{1}{2}} \right)}{\left\{ \left[\rho_{j+\frac{1}{2}} (R_{j+1} - R_j) \frac{2R_j + R_{j+1}}{3} \right] + \left[\rho_{j-\frac{1}{2}} (R_j - R_{j-1}) \frac{2R_j + R_{j-1}}{3} \right] \right\} / 2} \right\} \mathbf{e}_i^R,$$

where $\mathbf{e}_i^R = (\sin \varphi_i, \cos \varphi_i)^T$. Therefore, in discrete case acceleration is directed in ra-

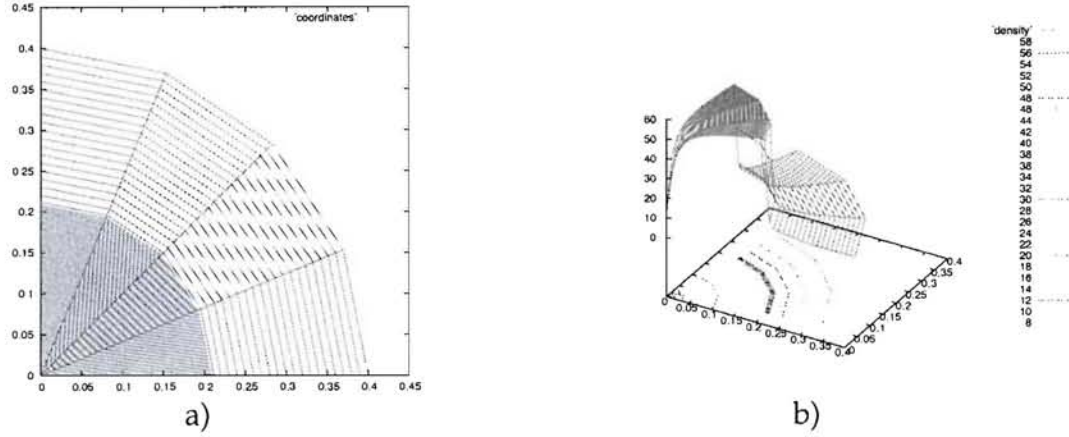


Figure 8. Noh Problem: a) Mesh, b) Density

dial direction, and its magnitude depends only on j , that is, momentum equation preserves spherical symmetry.

Equation for specific internal energy can be written as follows

$$\frac{d\varepsilon_{i+\frac{1}{2},j+\frac{1}{2}}}{dt} = \frac{1}{\rho_{j+\frac{1}{2}}} p_{j+\frac{1}{2}} \frac{1}{[(R_j)^2 + R_{j+1}R_j + (R_{j+1})^2]/3} \frac{(R_{j+1})^2 U_{j+1} - (R_j)^2 U_j}{R_{j+1} - R_j}.$$

To numerically demonstrate preservation of spherical symmetry we present results for so-called Noh's spherical problem. calculated in cylindrical geometry [3]. This problem has been used extensively to illustrate the difficulties of preserving spherical symmetry in cylindrical geometry. Initially the velocity is directed radially inward with a magnitude of 1.0, the density is unity, and the internal energy is zero. In Fig. 8 we present computational mesh at $t = 0.6$ and density. Numerical results clearly confirm our theory, that is, numerical solution preserves spherical symmetry exactly.

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