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

LA-UR 09-08130

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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. Although this formulation can be used for general polygonal meshes, we only describe it for a logically rectangular grid in this paper. We show that our discretization preserves spherical symmetry on polar equiangular meshes. The discretization conserves total energy 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. The general form of momentum equation for a Lagrangian fluid parcel $V(t)$ is

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

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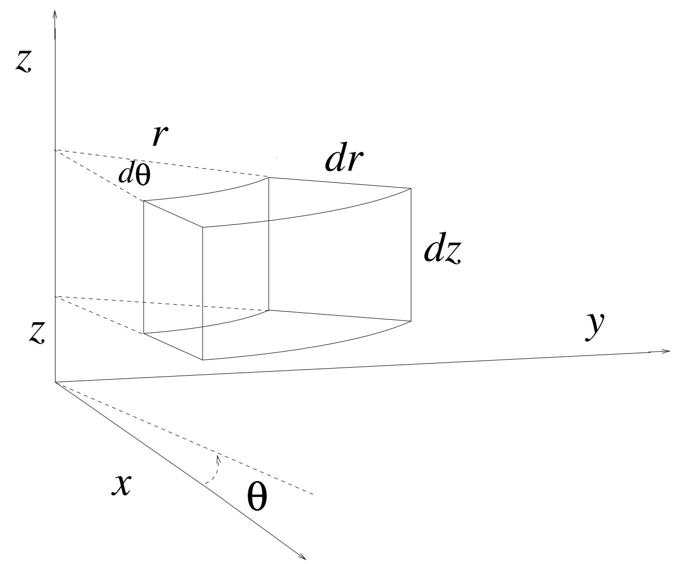


Figure 1. Control volume

If the general formula (1) is applied to the control volume presented in Fig. 1, one can obtain the following conservative form of the momentum equation in $r-z$ axisymmetric geometry

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

Here u and v are the r and z components of the velocity vector.

The equation for specific internal energy, ε, has the following form

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

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

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

The conservation law for total energy is

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

If initial and boundary conditions are specified appropriately, then the equations in cylindrical coordinates allow a spherically symmetric solution. That is, density, internal energy and pressure depend only upon the spherical radius ($R=\sqrt{r^2+z^2}$,

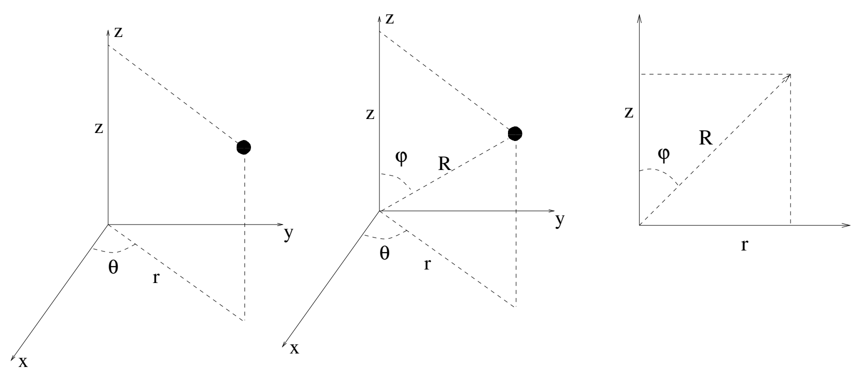


Figure 2. Cartesian - (x, y, z), cylindrical - $(r = \sqrt{x^2 + y^2}, z, \theta)$, and spherical Coordinates - $(R = \sqrt{r^2 + z^2}, \theta, \varphi)$

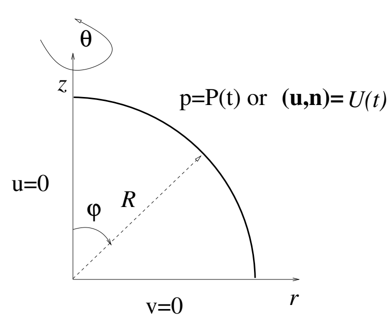
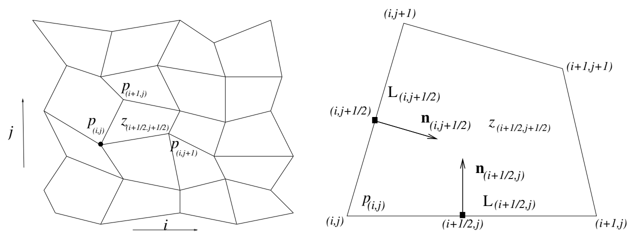


Figure 3. Boundary conditions for spherically symmetric problem



a) b)

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

$\rho(r,z) = \rho(R,t)$, $\varepsilon(r,z) = \varepsilon(R,t)$, $p(r,z) = p(R)$, and velocity can be represented as $u = U(R)\, \sin\varphi$, $v = U(R)\, \cos\varphi$ for coordinate systems 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 the radial direction and its amplitude depends only upon the spherical radius R:

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

The equation for internal energy has the following form:

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

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

2. COMPATIBLE STAGGERED DISCRETIZATION

For simplicity of presentation, 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 the 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: $d(m_z)/dt = 0$ with $m_z = \rho_z|_{t=0}\,\cdot V_z|_{t=0}$. 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 $\mathcal{E}_p = m_z\,\varepsilon_z$. 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 point mass, m_p, remains 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

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

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

$$\rho_z^p(t) = m_z^p / V_z^p(t)\,. \tag{9}$$

The generic compatible form of the discrete momentum and internal energy equations is

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

Therefore the spatial discretization is completely defined if we define subzonal masses m_z^p and subzonal forces 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 the 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 the change in total energy, $E = \mathcal{K} + \mathcal{E}$, is

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

which is the discrete form of total energy conservation.

3. DEFINITION OF SUBZONAL MASSES

The discretization of momentum equation that preserves spherical symmetry is based on the non-conservative ("Cartesian") form of the momentum equation

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

This is equivalent to (2) in the differential case.

A control volume derivation of the discrete "Cartesian" form of the momentum equation gives

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

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

$$\sum_{p\in\mathcal{P}(z)} (A^p_z)(t) = (A_z)(t)\,. \tag{12}$$

The discrete equation (11) is not in compatible form, therefore to construct a conservative discretization we need to define $(\rho^p_z)(t)$ and $(A^p_z)(t)$ in such a way that equation (11) can be rewritten in equivalent compatible form:

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

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 $\mathbf{f}^p_z$

$$m_p = r_p(t)\,\left(\sum_{z\in\mathcal{Z}(p)} (\rho^p_z)(t)\,(A^p_z)(t)\right)\,, \mathbf{f}^p_z(t) = r_p(t)\ (\mathbf{f}_{cart})^p_z\,(t)\,. \tag{14}$$

Using the notion of subzonal masses, we construct point point mass as follows

$$m_p = \sum_{z\in\mathcal{Z}(p)} m^p_z\,, \quad m^p_z = (\rho^p_z)(t)\, r_p(t)\,(A^p_z)(t) = (\rho^p_z)|_{t=0}\, r_p|_{t=0}\,(A^p_z)|_{t=0}\,. \tag{15}$$

This leads to a natural definition of subzonal volume

$$V^p_z(t) = r_p(t)\, A^p_z(t)\,. \tag{16}$$

Equation (8) leads to the following requirement for A^p_z

$$\sum_{p\in\mathcal{P}(z)} (V^p_z)(t) = \sum_{p\in\mathcal{P}(z)} (r_p)(t)\,(A^p_z)(t) = V_z(t)\,. \tag{17}$$

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

$$A^1_z = \frac{5\,A_{41} + 5\,A_{12} + A_{23} + A_{34}}{12}\,, \quad A^2_z = \frac{A_{41} + 5\,A_{12} + 5\,A_{23} + A_{34}}{12}$$
$$A^3_z = \frac{A_{41} + A_{12} + 5\,A_{23} + 5\,A_{34}}{12} \quad A^4_z = \frac{5\,A_{41} + A_{12} + A_{23} + 5\,A_{34}}{12}\,,$$

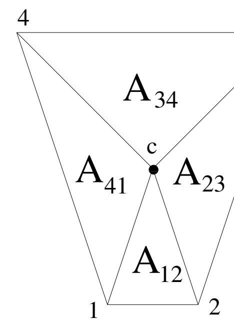


Figure 5. Volume Distribution. Geometric center of the quad is $r_c = (r_1 + r_2 + r_3 + r_4)/4$, $z_c = (z_1 + z_2 + z_3 + z_4)/4$

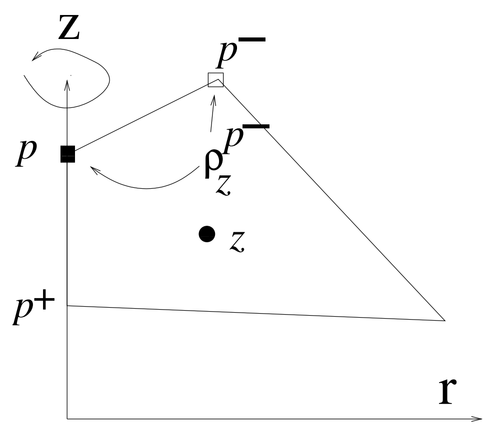


Figure 6. Definition of subzonal density for points on z axis

where corresponding triangles are shown in Fig. 5

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

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

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

It should be noted that such a definition of subzonal density does not affect the corresponding subzonal mass which remains zero because the corresponding subzonal volume is zero.

Now let us consider how this modification affects the logic of the compatible discretization. First, 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 the minimal consistency condition means that if $\mathbf{u}$ is constant then K_z should be exact. This is clearly true in our discretization because of the definition of subzonal volumes.

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

4. DISCRETE EQUATIONS ON LOGICALLY RECTANGULAR GRID

On logically rectangular grids, the discretization of "Cartesian" forces follows from the definition of the "Cartesian" gradient operator

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

Using notations for points and zones for such grids, we obtain the following expression for the subzonal forces

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

Similar discretization of momentum equation yields

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

Equation for internal energy looks as follows

$$m_{i+\frac{1}{2},j+\frac{1}{2}} \, \frac{\varepsilon^{n+1}_{i+\frac{1}{2},j+\frac{1}{2}} - \varepsilon^n_{i+\frac{1}{2},j+\frac{1}{2}}}{\Delta t} = -p_{i+\frac{1}{2},j+\frac{1}{2}} \, \left\{ \right.$$
$$\left[L_{i+\frac{1}{2},j+1} \, \mathbf{n}_{i+\frac{1}{2},j+1} \cdot \frac{r^n_{i,j+1} \, \mathbf{u}_{i,j+1} + r^n_{i+1,j+1} \, \mathbf{u}_{i+1,j+1}}{2} - L_{i+\frac{1}{2},j} \, \mathbf{n}_{i+\frac{1}{2},j} \cdot \frac{r^n_{i,j} \, \mathbf{u}_{i,j} + r^n_{i+1,j} \, \mathbf{u}_{i+1,j}}{2} \right] +$$
$$\left. \left[L_{i+1,j+\frac{1}{2}} \, \mathbf{n}_{i+1,j+\frac{1}{2}} \cdot \frac{r^n_{i+1,j} \, \mathbf{u}_{i+1,j} + r^n_{i+1,j+1} \, \mathbf{u}_{i+1,j+1}}{2} - L_{i,j+\frac{1}{2}} \, \mathbf{n}_{i,j+\frac{1}{2}} \cdot \frac{r^n_{i,j} \, \mathbf{u}_{i,j} + r^n_{i,j+1} \, \mathbf{u}_{i,j+1}}{2} \right] \right\}$$

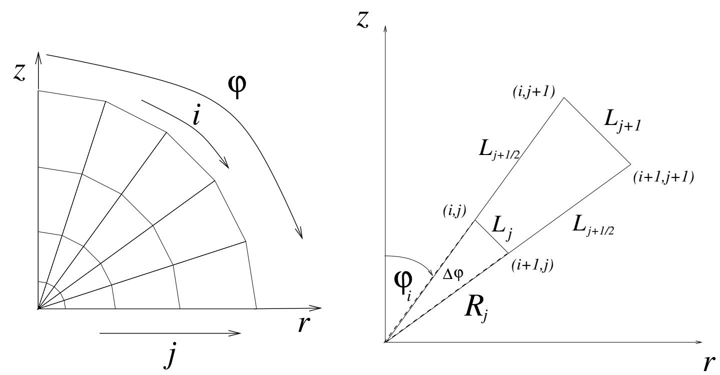


Figure 7. Equiangular polar mesh: a) Entire mesh, b) One cell

5. PRESERVATION OF SPHERICAL SYMMETRY ON AN 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 a mesh are defined as follows

$$r_{i,j} = R_j \, \sin\varphi_i \,, \quad z_{i,j} = R_j \, \cos\varphi_i \,; \quad i = 1, \cdots, I \,; j = 1, \cdots, J \,,$$
$$\varphi_i = (i-1)\, \Delta\varphi \,; \quad \Delta\varphi = \frac{\pi/2}{I-1} \,.$$

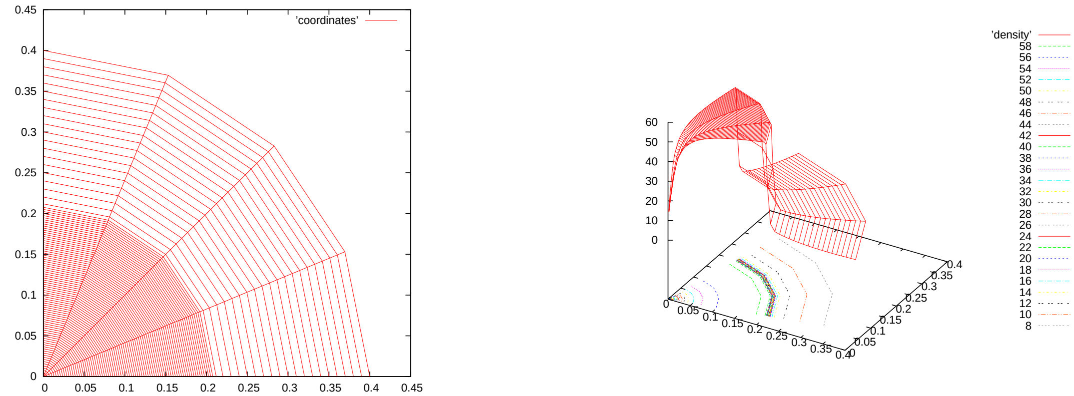
The statement of exact preservation of spherical symmetry on polar mesh can be formulated as follows. Corresponding components of the velocity are equal to zero on axis: $u_{1,j}(t) = 0$; $v_{I,j}(t) = 0$. Both components of the velocity are zero at the origin: $u_{1,1}(t) = v_{1,1}(t) = 0$. On the outer boundary, one can specify pressure as the function of the time $p_{i+1/2,J}(t) = P_{top}(t)$, or the 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 is 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 $u_{i,j}(t) = U_j(t)\, \sin\theta_i$ 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 a polar equiangular mesh, the momentum equation can be written in the following form

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



a) b)

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

where $\mathrm{e}_i^R = (\sin\varphi_i\,, \cos\varphi_i)^T$. Therefore, in the discrete case, acceleration is directed in the radial direction, and its magnitude depends only on j, that is, the momentum equation preserves spherical symmetry.

Similarly, the equation for specific internal energy also depends only on radius

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

To numerically demonstrate the preservation of spherical symmetry, we present results for the 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. The numerical results clearly confirm our theory; that is, the numerical solution preserves spherical symmetry exactly.

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