Energy Preserving Axisymmetric Finite Elements for Lagrangian Hydrodynamics

Truman E. Ellis

Joint work with: Veselin Dobrev (CASC), Tzanio Kolev* (CASC), and Robert Rieben* (WCI)
*Mentors

Institute for Scientific Computing Research
Lawrence Livermore National Laboratory
Livermore, CA 94550

ellis35@llnl.gov

August 3, 2010

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 LLNL-PRES-445911

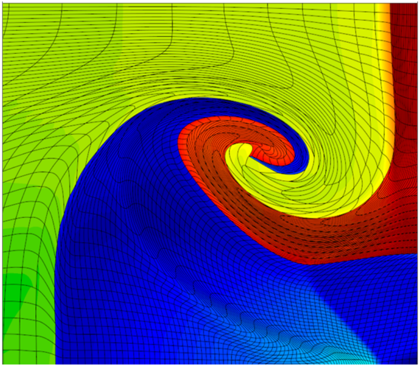
Introduction

Our goal is to improve the traditional staggered grid hydro (SGH) algorithms used to solve the Euler equations in multi-material ALE codes with respect to:

- Mesh imprinting / instabilities
- Symmetry preservation
- Total energy conservation
- Artificial viscosity

We consider a new approach[1] based on a generalized FEM treatment of the Euler equations in a Lagrangian frame with the following features:

- Curvilinear zone geometries
- Higher order field representations
- Exact discrete energy conservation by construction
- Reduces to classical SGH under simplifying assumptions
- Can be viewed as a high order extension of SGH



Curvilinear FEM Lagrangian calculation of shock triple point interaction.

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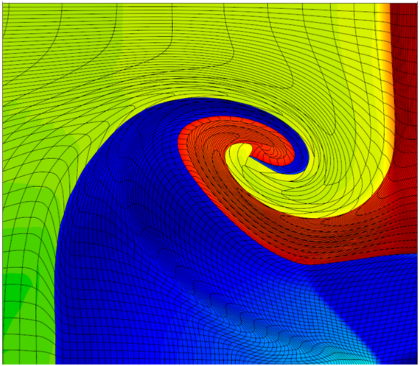

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Outline

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Euler Equations in a Lagrangian Frame

The Euler equations of gas dynamics in a Lagrangian reference frame can be written in differential form as:

Momentum Conservation: $\rho \frac{\mathrm{d}\vec{v}}{\mathrm{d}t} = -\nabla p + \ldots$

Mass Conservation: $\frac{1}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\nabla \cdot \vec{v}$

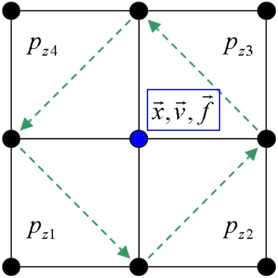
Energy Conservation: $\rho \frac{\mathrm{d}e}{\mathrm{d}t} = -p\nabla \cdot \vec{v} + \ldots$

Equation of State: $p = EOS(e, \rho)$

Equation of Motion: $\frac{\mathrm{d}\vec{x}}{\mathrm{d}t} = \vec{v}$

Typically, these equations are solved on a staggered spatial grid [1,2] where thermodynamic variables are approximated as piece-wise constants defined on zone centers and kinematic variables are defined on the nodes.

Spatial gradients are computed using finite volume and/or finite difference methods:

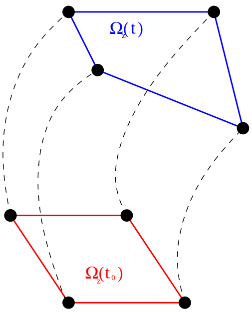


[1] R. Tipton, "CALE Lagrange Step, unpublished LLNL report, 1990

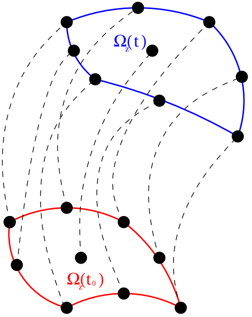
[2] M. Wilkins, "Calculations of Elastic-Plastic Flow, Methods of Computational Physics, 1964

Lagrangian Mesh Motion

After deformation in time, zones are reconstructed based on particle locations, thus defining the moved mesh.

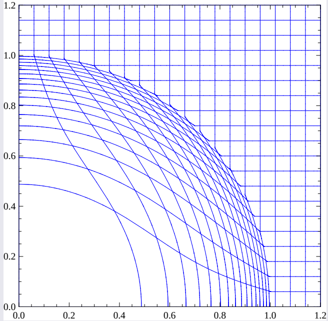


Q1 (Bi-Linear) Approximation



Q2 (Bi-Quadratic) Approximation

This reconstruction process has an inherent geometric error.



Initial Cartesian mesh deformed with the exact solution of the Sedov blast wave problem.

High order finite elements that use additional particle degrees of freedom are able to more accurately represent continuous deformations.

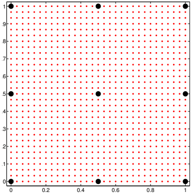
Outline

Kinematics

Velocity and position are approximated with high order finite elements using basis functions $\vec{w}_i$:

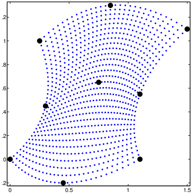
$$\vec{v}(\vec{x}, t) \approx \sum_{i}^{N_v} \mathbf{v}_i(t)\vec{w}_i(\vec{x})$$

Reference Space:



$$(\mathbf{J}_z)_{i,j} = \frac{\partial x_j}{\partial \hat{x}_i}$$

Physical Space:



The Position DOFs define the mapping from a reference element to physical space.

Weak formulation of the momentum conservation equation with a tensor artificial viscosity[1]:

$$\int_{\Omega(t)} \left(\rho \frac{\mathrm{d}\vec{v}}{\mathrm{d}t}\right) \cdot \vec{w}_i = \int_{\Omega(t)} (-\nabla p + \nabla \cdot \mu \nabla \vec{v}) \cdot \vec{w}_i = \int_{\Omega(t)} (p\mathbf{I} - \mu \nabla \vec{v}) : \nabla \vec{w}_i$$

Velocity Mass Matrix

$$\mathbf{M}_v = \int_\Omega \rho \mathbf{w}\mathbf{w}^T$$

Stress Tensor

$$\sigma = -p\mathbf{I} + \mu \nabla \vec{v}$$

Conservation of Momentum

$$\mathbf{M}_v \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\int_\Omega \sigma : \nabla \mathbf{w}$$

Equation of Motion

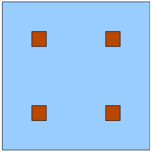
$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}$$

[1] Tz. Kolev, R. Rieben, "A tensor artificial viscosity using a finite element approach", Journal of Computational Physics 2009

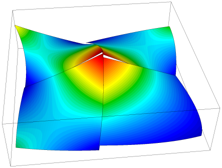
Thermodynamics

Internal energy is approximated from the set of discontinuous basis functions ϕ_i:

$$e(\vec{x}, t) \approx \sum_{i}^{N_e} \mathbf{e}_i(t)\phi_i(\vec{x})$$



Internal energy DOFs
on reference element



Patch of discontinuous Q_1 elements

Weak formulation of the energy conservation equation on zonal level

$$\int_{\Omega_z(t)} \left(\rho \frac{\mathrm{d}e}{\mathrm{d}t}\right) \phi_i = \int_{\Omega_z(t)} (\sigma : \nabla \vec{v})\, \phi_i$$

Energy Mass Matrix

$$\mathbf{M}_e = \int_\Omega \rho \boldsymbol{\phi} \boldsymbol{\phi}^T$$

Conservation of Energy

$$\mathbf{M}_e \frac{\mathrm{d}\mathbf{e}}{\mathrm{d}t} = \int_\Omega (\sigma : \nabla \vec{v})\, \boldsymbol{\phi}$$

Since the FEM space is discontinuous, $\mathbf{M}_e$ is block-diagonal and the above equation reduces to separate equations local to each zone.

Mass Conservation

In the Lagrangian description, the total mass of a zone is constant for all time:

$$\frac{\mathrm{d}m_z}{\mathrm{d}t} = 0, \quad m_z = \int_{\Omega_z(t)} \rho$$

Weak Formulation

We define high order zonal mass moments:

$$\mathbf{m}_{z,i} \equiv \int_{\Omega_z(t)} \rho \phi_i$$

Inserting the basis function expansion for density and writing in matrix vector form:

$$\mathbf{m}_z = \mathbf{M}_z^\rho \boldsymbol{\rho}_z \text{ where } (\mathbf{M}_z^\rho)_{i,j} \equiv \int_{\Omega_z(t)} \phi_i \phi_j$$

We therefore generalize zonal mass conservation to the high order moments:

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{M}_z^\rho \boldsymbol{\rho}_z) = 0}$$

Strong Formulation

If we impose the stronger condition:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega_z(t)} \rho \psi = 0 \quad \text{for } \textbf{any} \text{ function } \psi$$

then we obtain the
strong mass conservation principle:

$$\boxed{\rho(t)|\mathbf{J}(t)| = \rho(t_0)|\mathbf{J}(t_0)|}$$

Furthermore, this implies that the mass matrices are constant for all time:

$$\frac{\mathrm{d}\mathbf{M}_v}{\mathrm{d}t} = 0, \quad \frac{\mathrm{d}\mathbf{M}_e}{\mathrm{d}t} = 0$$

Note that both generalizations reduce to classical SGH for the case of a single, constant moment

Generalized Corner Forces

We can consolidate our calculations by defining a Generalized Corner Force matrix.

$$(\mathbf{F})_{ij} = \int_{\Omega(t)} (\sigma : \nabla \vec{w}_i)\, \phi_j$$

We can rewrite our equations:

Conservation of Momentum

$$\mathbf{M}_v \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\mathbf{F} \cdot \mathbf{1}$$

Conservation of Energy

$$\mathbf{M}_e \frac{\mathrm{d}\mathbf{e}}{\mathrm{d}t} = \mathbf{F}^T \cdot \mathbf{v}$$

Density is evaluated pointwise via the strong mass conservation principle.
Pressure is evaluated point wise using the density and energy (EOS).

Strong mass conservation implies exact semi-discrete energy conservation:

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\int_{\Omega(t)} \rho \frac{|\vec{v}|^2}{2} + \rho e\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathbf{v} \cdot \mathbf{M}_v \cdot \mathbf{v}}{2} + \mathbf{1} \cdot \mathbf{M}_e \cdot \mathbf{e}\right) = 0.$$

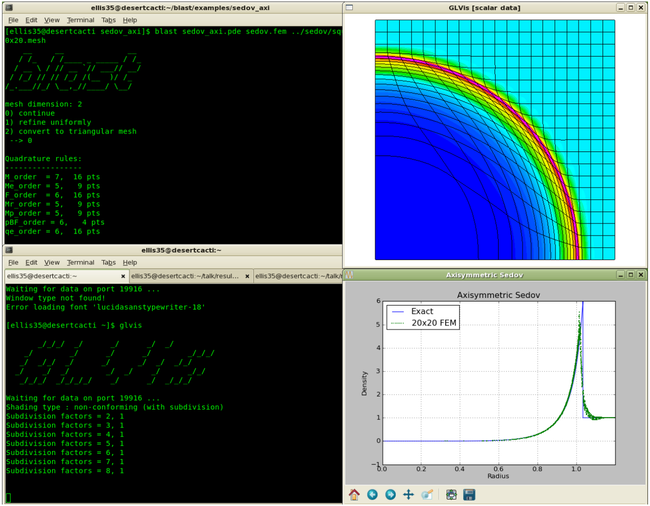
Research Codes

BLAST C++ High order FEM Lagrangian hydrocode

MFEM Modular C++ finite element library

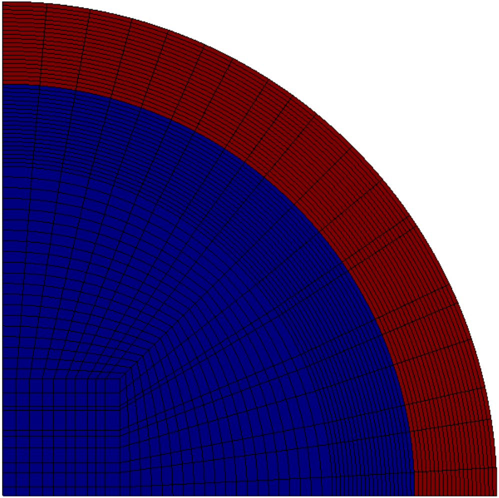
GLVis OpenGL visualization tool (curvilinear zones, high-order fields)

MPLVis Python scriptable Matplotlib plotting tool



ICF-like Results in Cartesian Coordinates

- Simple 2D implosion of a cylindrical shell of ideal gas using an ICF like pressure drive. The interface between the high density and low density regions is subject to both Richtmyer-Meshkov (RM) and Rayleigh-Taylor (RT) instabilities. [1]
- Random angular sub-divisions
- Results computed with BLAST
- Q2-Q1 spatial discretization
- RK2Avg temporal discretization ensuring exact total energy conservation

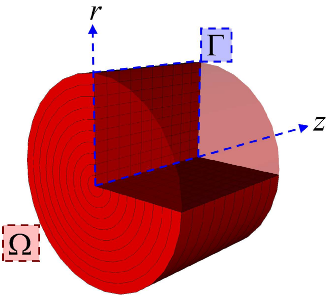


[1] S. Galera, P-H. Maire, J. Breil, "A two-dimensional unstructured cell-centered multi-material ALE scheme using VOF interface reconstruction". JCP Preprint

Outline

Axisymmetric Hydro

Axisymmetric simulations are attractive computationally



Compatibility and convergence are essential for a predictive computational capability.

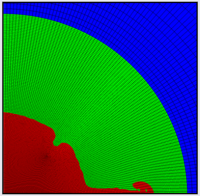
Symmetry breaking and lack of energy conservation lead to non-physical results

Axisymmetric ICF Test

ICF implosion with radial pressure drive

Initial unstructured butterfly mesh

This jet is 100% numerical and gets worse as mesh is refined in space



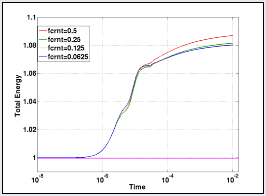
Axisymmetric Sedov Test

Sedov test in axi-symmetric mode

Total energy should be 1.0 for all time

Traditional PdV energy update is not conservative in r-z geometry

Around 8.5% artificial gain in energy. Converges under time refinement, but not to the correct value



Axisymmetric Momentum Equation

Rewriting the 3D momentum equation with a tensor artificial viscosity,

$$\int_{\Omega(t)} \left(\rho \frac{\mathrm{d}\vec{v}}{\mathrm{d}t}\right) \cdot \vec{w}_i = \int_{\Omega(t)} (p\mathbf{I} - \mu \nabla \vec{v}) : \nabla \vec{w}_i = -\int_{\Omega(t)} \sigma : \nabla \vec{w}_i$$

Reducing this to the axisymmetric cut plane Γ,

$$2\pi \int_{\Gamma(t)} r \left(\rho \frac{\mathrm{d}\vec{v}}{\mathrm{d}t}\right) \cdot \vec{w}_i = -2\pi \int_{\Gamma(t)} r\sigma_{rz} : \nabla_{rz} \vec{w}_i$$

Applying the cylindrical gradient operator $\nabla_{rz} f = \frac{\partial f}{\partial r}\vec{e}_r + \frac{1}{r}\frac{\partial f}{\partial \theta}\vec{e}_\theta + \frac{\partial f}{\partial z}\vec{e}_z$

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$$+\frac{1}{r}\left(\frac{\partial v_r}{\partial \theta}\vec{e}_r \otimes \vec{e}_\theta + v_r \frac{\partial \vec{e}_r}{\partial \theta} \otimes \vec{e}_\theta + \frac{\partial v_z}{\partial \theta}\vec{e}_z \otimes \vec{e}_\theta + \frac{\partial \vec{e}_z}{\partial \theta}\vec{v}_z \otimes \vec{e}_\theta\right)$$

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Axisymmetric Momentum Equation

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Recall

$$\vec{e}_r = (\cos\theta, \sin\theta, 0)\,, \quad \vec{e}_\theta = (-\sin\theta, \cos\theta, 0)\,, \quad \vec{e}_z = (0,0,1)$$

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Thus, the axisymmetric velocity gradient is

$$\nabla_{rz}\vec{v} = \begin{pmatrix} \frac{\partial v_z}{\partial z} & \frac{\partial v_z}{\partial r} & 0 \\ \frac{\partial v_r}{\partial z} & \frac{\partial v_r}{\partial r} & 0 \\ 0 & 0 & \frac{v_r}{r} \end{pmatrix}_{z-r-\theta} = \begin{pmatrix} \nabla_{2d}\vec{v} & 0 \\ 0 & \frac{v_r}{r} \end{pmatrix}$$

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Reducing this to the axisymmetric cut plane Γ,

$$\cancel{2\pi} \int_{\Gamma(t)} r \left(\rho \frac{\mathrm{d}\vec{v}}{\mathrm{d}t}\right) \cdot \vec{w}_i = -\cancel{2\pi} \int_{\Gamma(t)} r \sigma_{rz} : \nabla_{rz} \vec{w}_i$$

For $\sigma = -p\mathbf{I} + \mu \nabla \vec{v}$, the axisymmetric stress tensor is

$$\sigma_{rz} = \begin{pmatrix} -p\mathbf{I} + \mu \nabla_{2d} \vec{v} & 0 \\ 0 & -p + \mu \frac{v_r}{r} \end{pmatrix}$$

The axisymmetric momentum equation becomes

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Axisymmetric Momentum Equation

Rewriting the 3D momentum equation with a tensor artificial viscosity,

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$$= -\int_{\Gamma(t)} r \left[(\sigma_{2d} : \nabla_{2d} \vec{w}_i) - p \frac{w_r}{r} + \mu \frac{v_r w_r}{r^2} \right]$$

Axisymmetric Momentum Equation

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$$= -\int_{\Gamma(t)} r(\sigma_{2d} : \nabla_{2d} \vec{w}_i) - p w_r + \mu \frac{v_r w_r}{r}$$

Axisymmetric Momentum Equation

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$$= -\int_{\Gamma(t)} r(\sigma_{2d} : \nabla_{2d} \vec{w}_i) - p w_r + \mu \frac{v_r w_r}{r}$$

Semi-discrete Axisymmetric Method

Axisymmetric mass matrices $\mathbf{M}_v^{rz} = \int_{\Gamma(t)} r\rho \mathbf{w}\mathbf{w}^T \qquad \mathbf{M}_e^{rz} = \int_{\Gamma(t)} r\rho \boldsymbol{\phi}\boldsymbol{\phi}^T$

Axisymmetric generalized corner force matrix

$$(\mathbf{F}^{rz})_{ij} = \int_{\Gamma(t)} r\left(\sigma_{rz} : \nabla_{rz}\vec{w}_i\right)\phi_j$$

We can rewrite our equations:

Conservation of Momentum

$$\mathbf{M}_v^{rz}\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\mathbf{F}^{rz}\cdot\mathbf{1}$$

Conservation of Energy

$$\mathbf{M}_e^{rz}\frac{\mathrm{d}\mathbf{e}}{\mathrm{d}t} = \left(\mathbf{F}^{rz}\right)^T\cdot\mathbf{v}$$

The axisymmetric strong mass conservation principle reads $r(t)\rho(t)|\mathbf{J}(t)| = r(t_0)\rho(t_0)|\mathbf{J}(t_0)|$ which implies

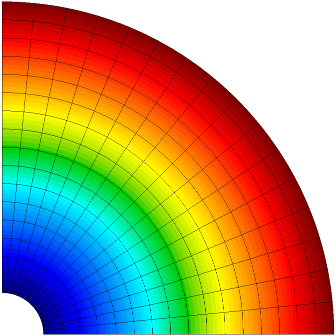
$$\frac{\mathrm{d}\mathbf{M}_v^{rz}}{\mathrm{d}t} = 0, \qquad \frac{\mathrm{d}\mathbf{M}_e^{rz}}{\mathrm{d}t} = 0$$

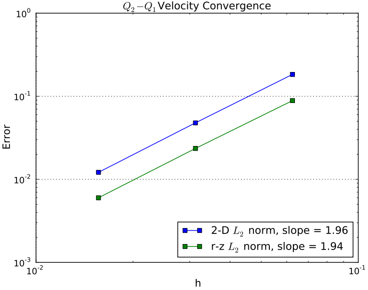
and the exact axisymmetric semi-discrete energy conservation:

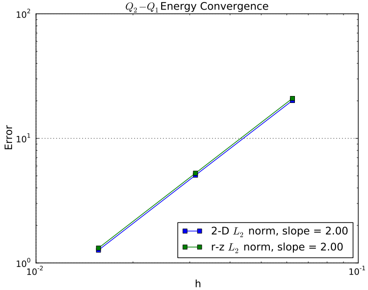
$$\frac{\mathrm{d}E^{rz}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\int_{\Omega(t)}\rho\frac{|\vec{v}|^2}{2} + \rho e\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(2\pi\int_{\Gamma(t)} r\rho\frac{|\vec{v}|^2}{2} + r\rho e\right) = 0.$$

Outline

Axisymmetric Coggeshall Q2-Q1 Convergence

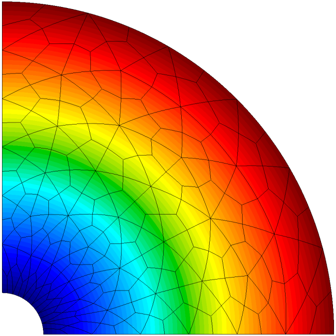




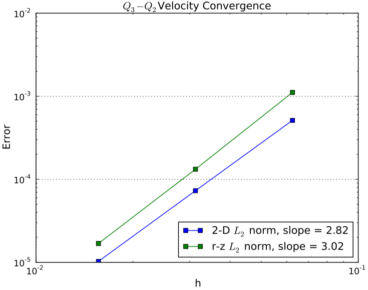


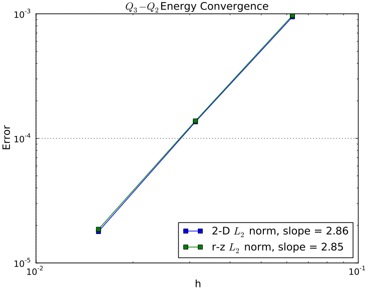
- Coggeshall[a] self-similar adiabatic compression problem # 1
- Curved structured annular mesh
- Q2-Q1 Finite Elements
- RK2Avg time step

[a] S. Coggeshall, "Analytic solutions of hydrodynamics equations," Physics of Fluids, 1991



- Coggeshall[a] self-similar adiabatic compression problem # 1
- Curved unstructured annular mesh
- Q3-Q2 Finite Elements
- RK4 time step

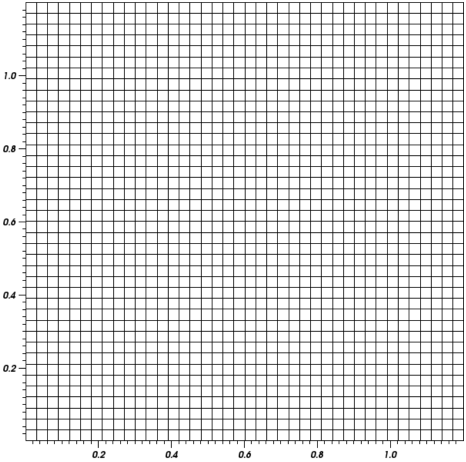




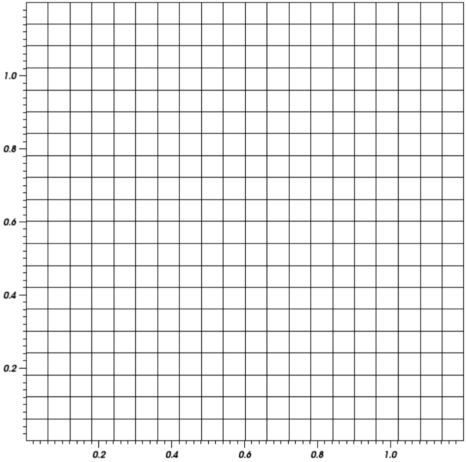
[a] S. Coggeshall, "Analytic solutions of hydrodynamics equations," Physics of Fluids, 1991

Axisymmetric Sedov Explosion

40x40 Lagrangian SGH - Density



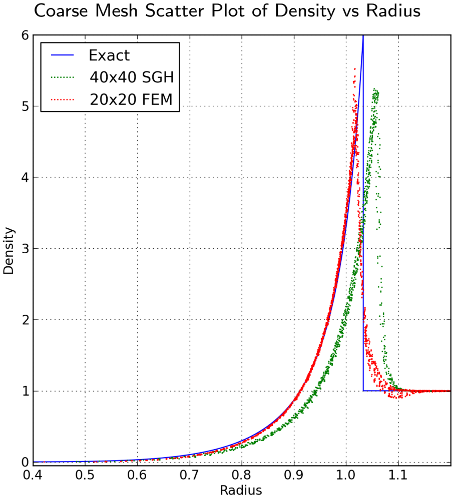
20x20 Lagrangian FEM - Density

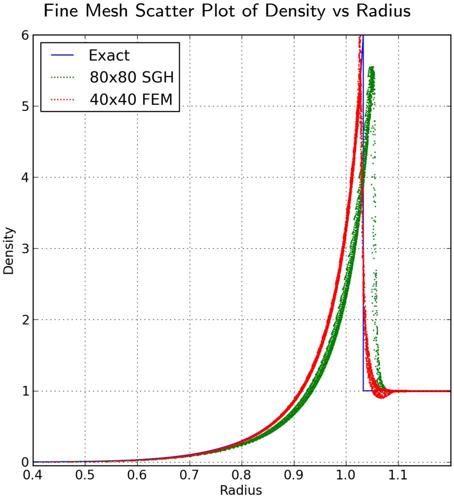


- Symmetry is not preserved
- Mesh distorted near the origin

- Symmetry is preserved
- Curvilinear zones match physics

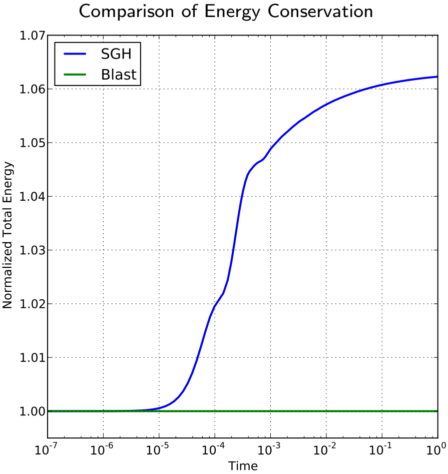
Axisymmetric Sedov - Scatter Plots



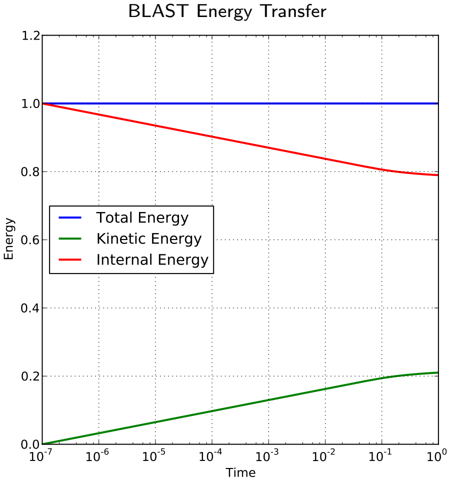


- SGH shock is too fast
- FEM is good with only 20x20 zones
- SGH does not improve under refinement
- FEM matches exact solution very closely

Axisymmetric Sedov - Energy Conservation



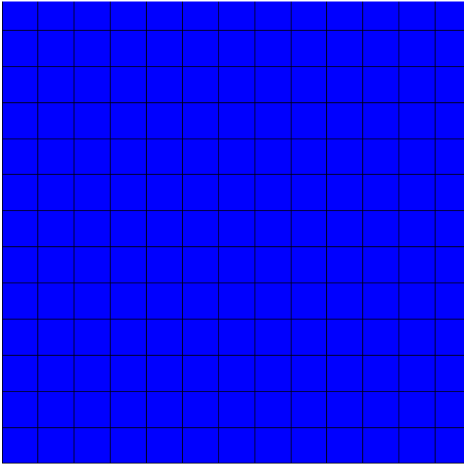
- SGH gains 6% energy
- BLAST conserves energy to machine precision



- BLAST converts IE to KE without loss

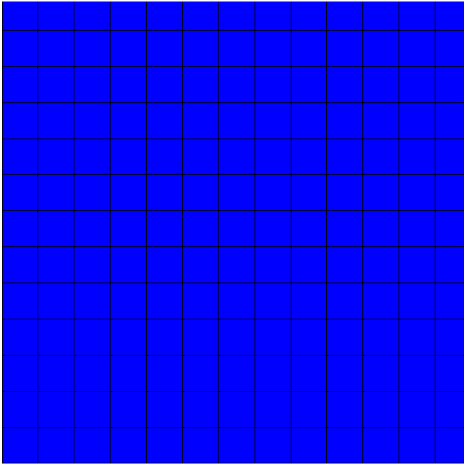
Axisymmetric Noh Implosion

32x32 Lagrangian SGH



- Symmetry is not preserved
- Mesh distorted near the origin

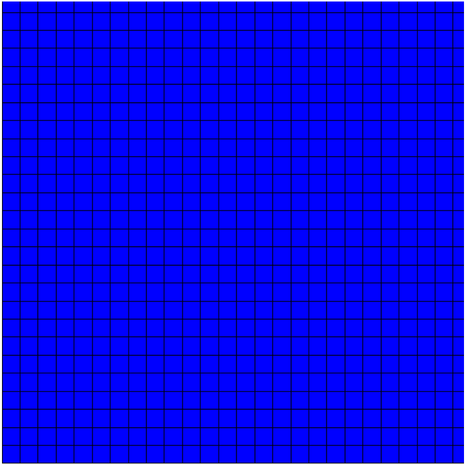
32x32 Lagrangian FEM



- Symmetry is preserved
- Wall heating is typical for Lagrangian methods

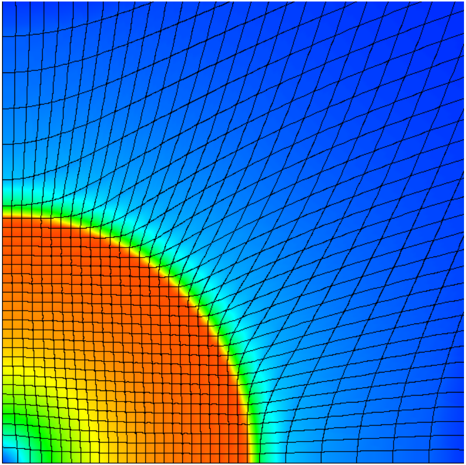
Axisymmetric Noh Implosion

64x64 Arbitrary Lagrangian Eulerian SGH



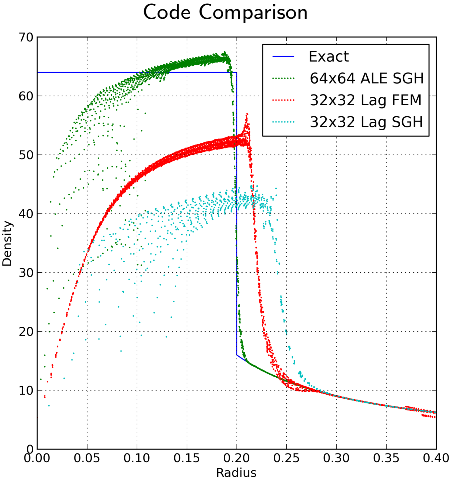
- ALE fixes mesh
- Energy jets from wall heating

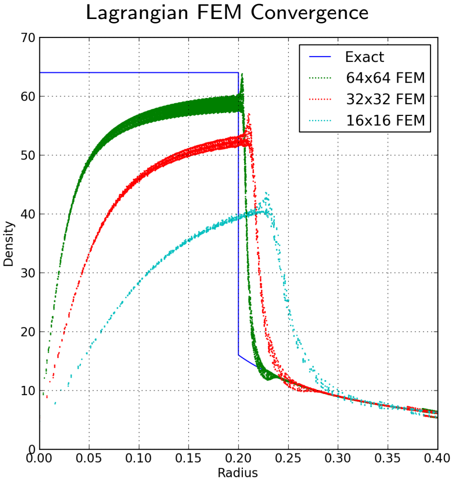
32x32 Lagrangian FEM



- Symmetry is preserved
- Wall heating is typical for Lagrangian methods

Axisymmetric Noh - Symmetry Preservation

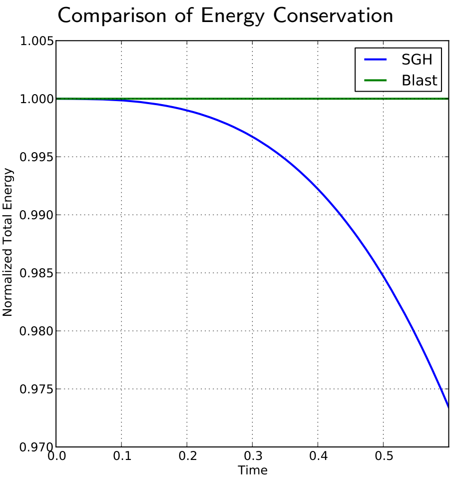




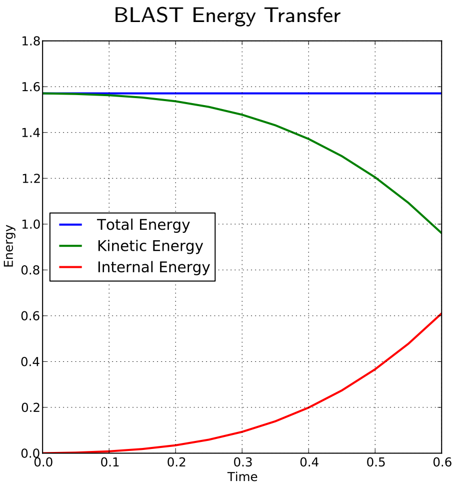
- SGH does not preserve symmetry
- ALE gives good shock prediction
- FEM preserves symmetry

- FEM converges to correct solution
- Wall heating is typical for Lagrangian methods

Axisymmetric Noh - Energy Conservation

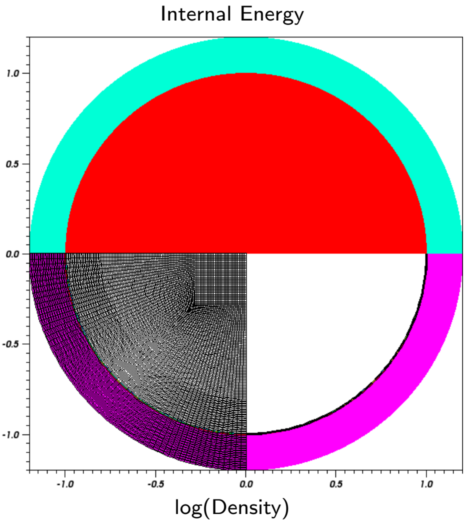


- ALE SGH loses 3% energy
- BLAST conserves energy to machine precision

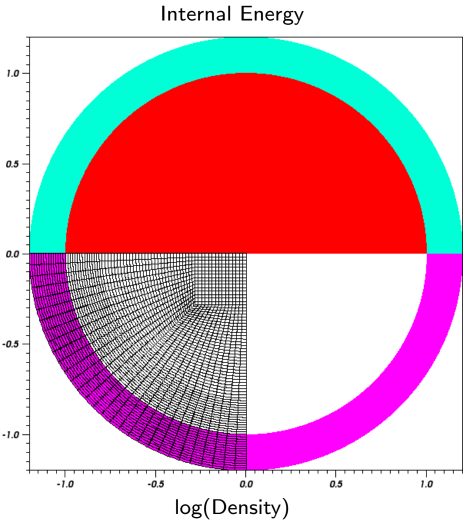


- BLAST converts KE to IE without loss

Simple Velocity Driven ICF-like Test



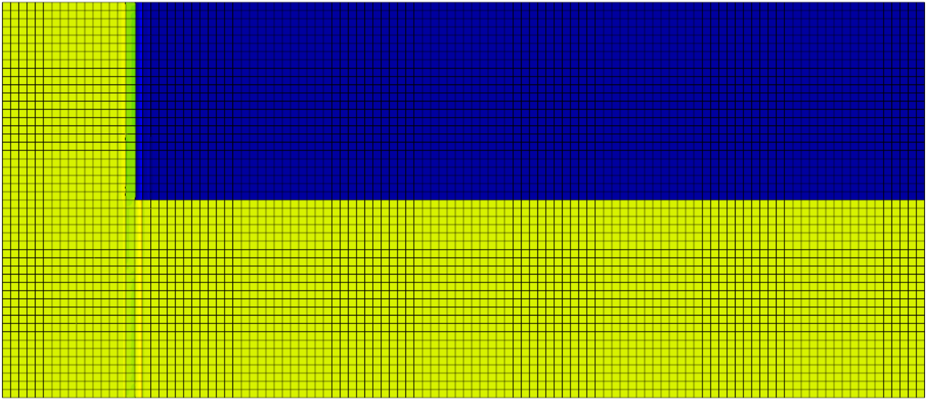
ALE Staggered Grid Hydro



Pure Lagrangian FEM

Axisymmetric Triple Point Shock

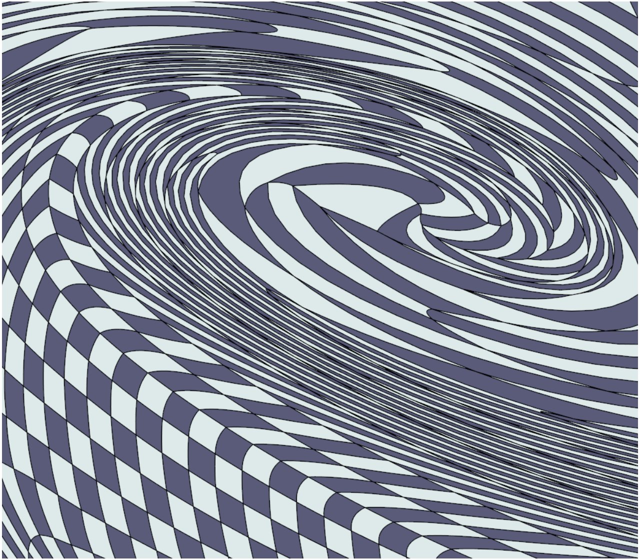
Density



- More complicated shock flow
- Multi-material Riemann problem
- No spurious features near the axis of symmetry
- Demonstrates robustness of higher order FEM

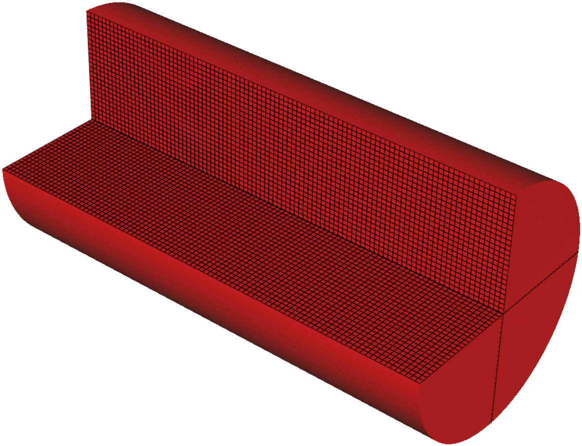
Axisymmetric Triple Point Shock

- High aspect ratios
- Curved zones
- Impossible to represent with straight edges

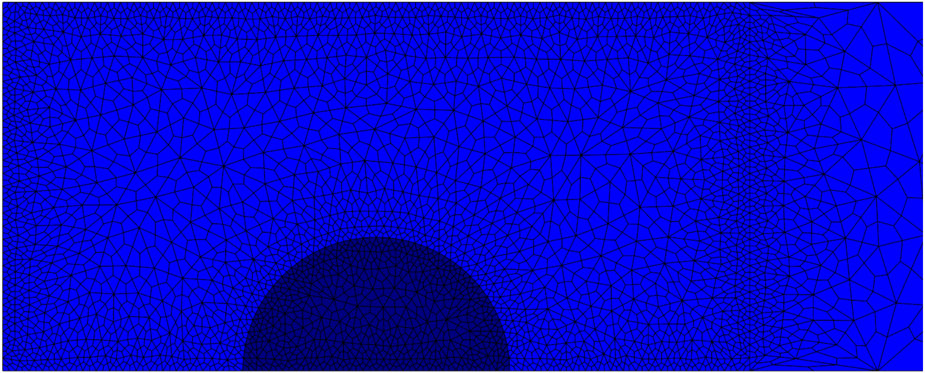


Closeup of skewed zones in the triple point shock

Axisymmetric Triple Point Shock



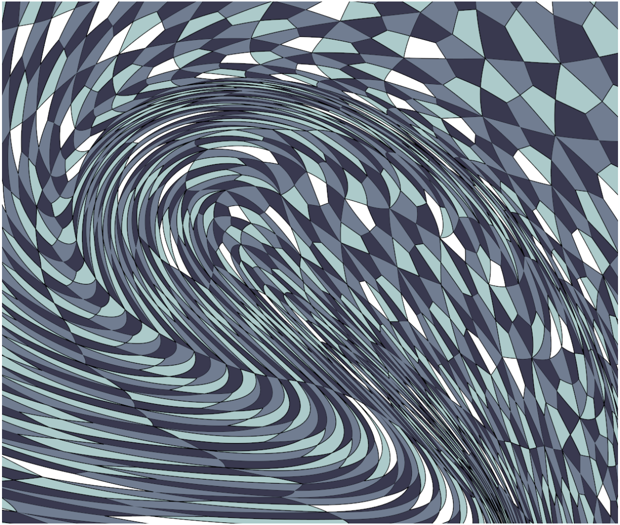
Axisymmetric Helium Bubble



- Unstructured mesh with local refinement
- Shock remains straight before impact
- No spurious features near the axis of symmetry
- Demonstrates robustness of higher order FEM

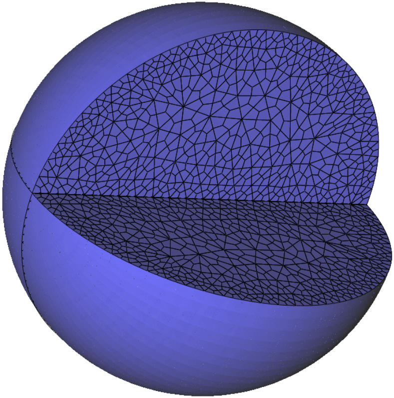
Axisymmetric Helium Bubble

- High aspect ratios
- Curved zones
- Impossible to represent with straight edges



Closeup of skewed zones in the helium bubble

Axisymmetric Helium Bubble



Conclusions

We have developed a general energy-conserving, high order finite element discretization of the Euler equations in a Lagrangian frame.

Benefits of high order elements:

- The ability to more accurately capture geometrical features of a flow region using curvilinear zones
- Elimination of the need for ad-hoc hourglass filters
- Sharper resolution of a shock front for a given mesh resolution
- The ability to represent a shock within a single zone
- Substantial reduction in mesh imprinting for shock wave propagation not aligned with the computational mesh

In this talk, we have extended this method to axisymmetric problems while simultaneously conserving energy and preserving symmetry

Our axisymmetric formulation:

- Conserves energy by construction
- Demonstrates improved symmetry preservation
- Is robust to complicated problem geometries