A 3D Arbitrary Lagrangian Eulerian (ALE) hydrodynamic approach for tetrahedral meshes

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We seek to develop 3D ALE hydrodynamic algorithms for unstructured tetrahedral meshes

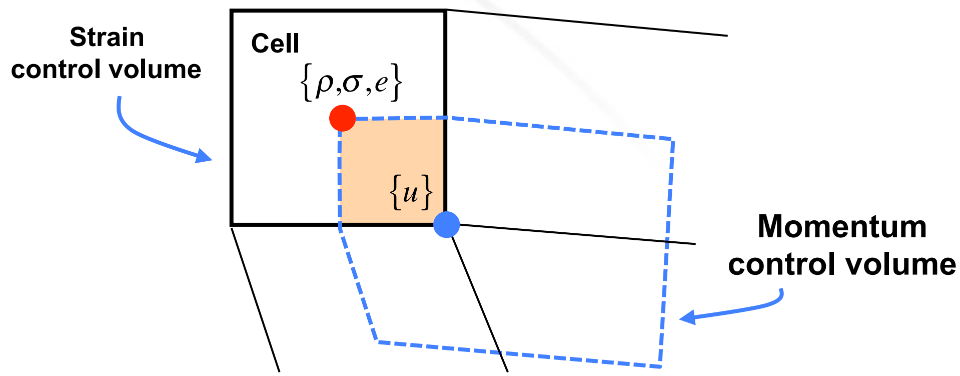
- We are exploring a range of topics related to computational hydrodynamics:
  - Efficient computing on advanced computing architectures
  - Automatic mesh refinement (AMR) and mesh coarsening
  - Multiple materials
  - Strength
  - Failure
  - Materials with phase transition
  - Eulerian, Lagrangian, and ALE hydro methods

Outline

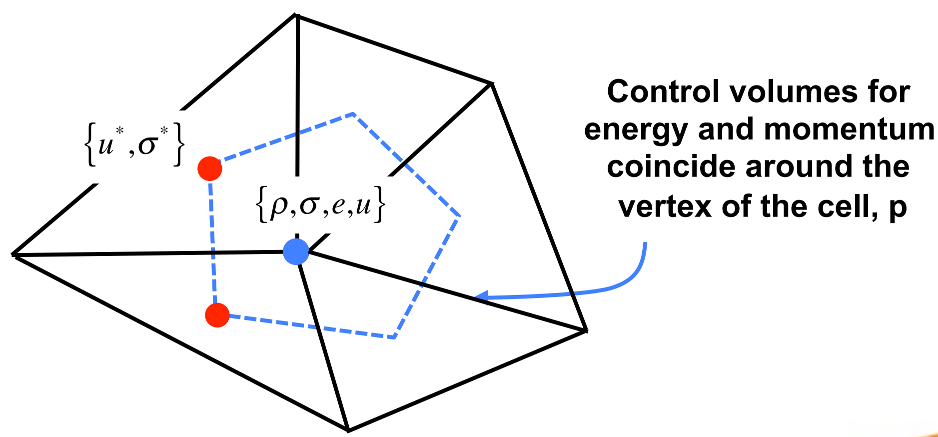
- Overview of ALE hydrodynamic algorithm
- Lagrangian hydrodynamic test problems
- ALE hydrodynamic test problems

Control volumes (CV) are used to enforce conservation

- Staggered grid hydro (SGH)
  - Momentum control volume (CV) is staggered with respect to the strain/energy volumes



- Point-centered hydro (PCH)
  - CVs coincide (i.e. spatially collocated)
  - **The approach used in this work is PCH**



The PCH approach has a rich history of research

- The objective of this research is to develop an ALE approach suitable for modeling shock problems on tetrahedron meshes
- The PCH approach is a viable option
  - Previous research in Lagrangian PCH includes:
    - Crowley 1971, Fritts and Boris 1979, Crowley 1985, Clark 1988, Gittings 1990, Sahota 1990, Scovazzi 2010, and Scovazzi 2013
  - Previous research in Eulerian PCH includes:
    - Waltz 2004, Waltz et. al. 2013
  - Previous research in ALE PCH:
    - Waltz et. al. 2013
- In this presentation, we present a new ALE PCH approach that is <u>essentially</u> Lagrangian when the mesh moves at the fluid velocity and is Eulerian when the mesh is stationary
  - The approach reduces to pure Lagrangian motion in the limit of the mesh size going to zero or if the flow is linear

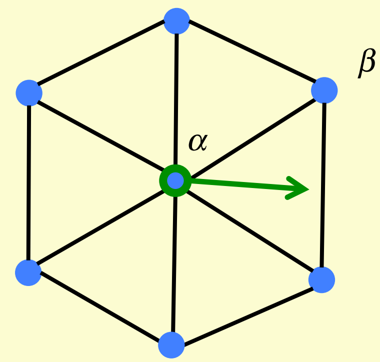
Why essentially Lagrange? A volume error arises when the mesh is moved at the fluid velocity rather than the contact wave velocity

PCH volume definitions:

1) $\dfrac{\Delta V_\alpha}{\Delta t} = \sum_{i \in \alpha} \left(\mathbf{S}_i \cdot \mathbf{u}_e \right) \qquad \mathbf{u}_e = \dfrac{1}{2}\left(\mathbf{u}_\alpha + \mathbf{u}_\beta \right)$

2) $V_\alpha = \dfrac{1}{4} \sum_{z \in \alpha} V_z$ **Lumped volume**

The Error:
There will be no volume change when the node alpha is accelerating or decelerating and the beta nodes are moving at a constant velocity. The Sod problem will expose this error. (Esmond and Thurber 2013)



Proof of error with definition (1):

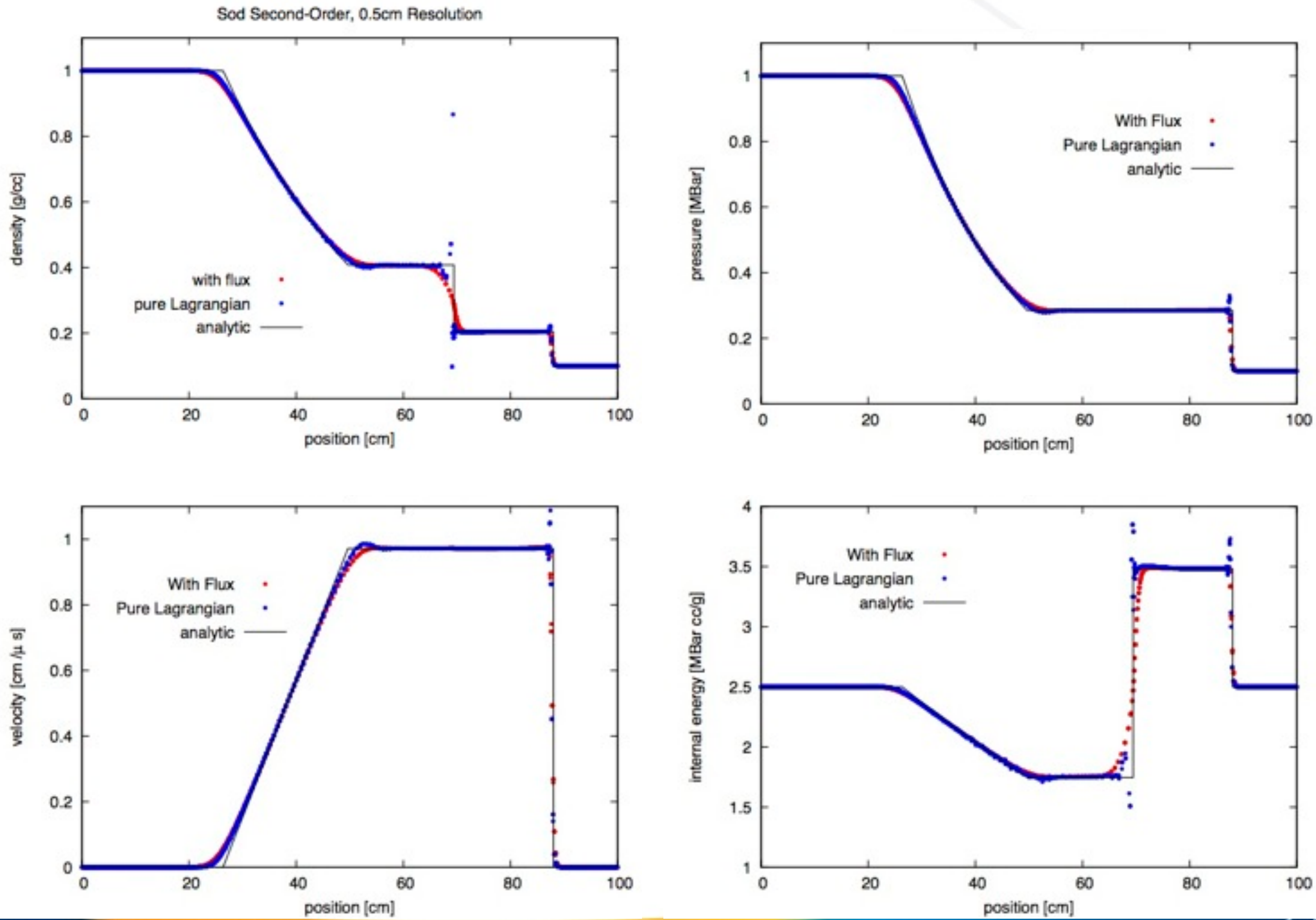
$$\frac{\Delta V_\alpha}{\Delta t} = \sum_{i \in \alpha} \left(\mathbf{S}_i \cdot \frac{1}{2}\left(\mathbf{u}_\alpha + \mathbf{u}_\beta \right) \right) = \frac{1}{2} \sum_{i \in \alpha} \mathbf{S}_i \cdot \mathbf{u}_\alpha + \frac{1}{2} \sum_{i \in \alpha} \mathbf{S}_i \cdot \overbrace{\mathbf{u}_\beta}^{\mathbf{u}_\beta = \text{constant}} = \frac{1}{2} \Big(\underbrace{\cancel{\sum_{i \in \alpha} \mathbf{S}_i}}_{=0} \Big) \cdot \mathbf{u}_\alpha + \frac{1}{2} \Big(\underbrace{\cancel{\sum_{i \in \alpha} \mathbf{S}_i}}_{=0} \Big) \cdot \mathbf{u}_\beta = 0$$

The volume change will always be equal to zero for any mesh topology, any mesh surface normal definition, and any velocity.

Proof of error with definition (2):

$$\frac{\Delta V_\alpha}{\Delta t} = \frac{1}{4} \sum_{z \in \alpha} \left(\sum_{i \in z} \mathbf{A}_i \cdot \mathbf{u}_p \right) = \frac{1}{4} \sum_{z \in \alpha} \left(\sum_{i(\alpha) \in z} \mathbf{A}_i \cdot \mathbf{u}_\alpha + \sum_{i(\beta) \in z} \mathbf{A}_i \cdot \overbrace{\mathbf{u}_\beta}^{\mathbf{u}_\beta = \text{constant}} \right) = \frac{1}{4} \sum_{z \in \alpha} \left(\Big(\underbrace{\cancel{\sum_{i(\alpha) \in z} \mathbf{A}_i}}_{=0} \Big) \cdot \mathbf{u}_\alpha + \Big(\underbrace{\cancel{\sum_{i(\beta) \in z} \mathbf{A}_i}}_{=0} \Big) \cdot \mathbf{u}_\beta \right) = 0$$

The volume error generates numerical oscillations at the contact discontinuity in the Sod problem and prevents convergence



Mesh = 0.5 cm

Additional advective fluxes are used to remove the volume error

- Lagrangian CCH avoids this volume error by evolving the control volume vertices at the contact wave speed instead of the average of the nodal velocities

$$\frac{\Delta V_\alpha^{CCH}}{\Delta t} = \sum_{i\in\alpha}\left(\mathbf{S}_i \cdot \mathbf{u}_z^*\right)$$

- The concept is to evolve the mesh at a velocity close to the Riemann velocity and then “remap” back to the PCH control volume location
- Rusanov fluxes as used in this work

$$\frac{\Delta V_\alpha}{\Delta t} = \sum_{i\in\alpha}\left(\mathbf{S}_i \cdot \left(\mathbf{u}_i^* - \delta\mathbf{u}_i\right)\right)$$

The actual PCH CV is moving at a drift velocity relative to the contact wave speed

$$\frac{\Delta V_\alpha^{Adv}}{\Delta t} = \sum_{i\in\alpha}\left(\mathbf{S}_i \cdot \delta\mathbf{u}_i\right) \approx \sum_{i\in\alpha}\left(\mathbf{S}_i \cdot \underline{\mathbf{s}_i a_i}\right)$$

Advected volume

Mass: $f_i^{\rho} = \underline{\mathbf{s}_i a_i}\left(\rho_i^* - \rho_c\right)$

Momentum: $f_i^{\rho\mathbf{u}} = \underline{\mathbf{s}_i a_i}\left(\rho_i^* \mathbf{u}_i^* - \rho_c \mathbf{u}_c\right)$

Total energy: $f_i^{\rho j} = \underline{\mathbf{s}_i a_i}\left(\rho_i^* j_i^* - \rho_c j_c\right)$

$$\mathbf{u}_i^* = \mathbf{u}_e + \delta\mathbf{u}_i \approx \mathbf{u}_e + a_i$$

a_i is an approximation of the shock speed

The discrete conservation equations contain an extra flux to correct the volume error, which goes to zero in the limit of a zero mesh size or a linear flow

Analytic equations

$$\frac{d}{dt}\int_V \rho dV + \oint_{\partial V} (d\mathbf{S}\cdot \rho(\mathbf{u}-\mathbf{w})) = 0$$

$$\frac{d}{dt}\int_V \rho \mathbf{u} dV + \oint_{\partial V} (d\mathbf{S}\cdot \rho\mathbf{u}(\mathbf{u}-\mathbf{w})) = \oint_{\partial V} (d\mathbf{S}\cdot \boldsymbol{\sigma})$$

$$\frac{d}{dt}\int_V \rho j dV + \oint_{\partial V} (d\mathbf{S}\cdot \rho j(\mathbf{u}-\mathbf{w})) = \oint_{\partial V} (d\mathbf{S}\cdot \boldsymbol{\sigma}\cdot\mathbf{u})$$

Discrete approximation

$$\frac{\Delta U_\alpha V_\alpha}{\Delta t} = \sum_{i\in\alpha} S_i \cdot F_i \qquad F_i = \begin{bmatrix} \rho_i^*\left(\mathbf{w}_i - \mathbf{u}_i\right) \\ \sigma_c^* + \rho_i^*\mathbf{u}_i^*\left(\mathbf{w}_i - \mathbf{u}_i\right) \\ \sigma_c^*\cdot\mathbf{u}_z^* + \rho_i^* j_i^*\left(\mathbf{w}_i - \mathbf{u}_i\right) \end{bmatrix} + \mathbf{s}_i a_i \begin{array}{c} \underbrace{\begin{bmatrix} \rho_i^* - \rho_c \\ \rho_i^*\mathbf{u}_i^* - \rho_c\mathbf{u}_c \\ \rho_i j_i^* - \rho_c j_c^* \end{bmatrix}} \end{array} \begin{array}{l} \textbf{mass} \\ \textbf{momentum} \\ \textbf{total energy} \end{array}$$

Rusanov fluxes ensure numerical stability and fix a volume error

2nd-order accuracy is achieved by reconstructing the fields with linear Taylor-Series expansions

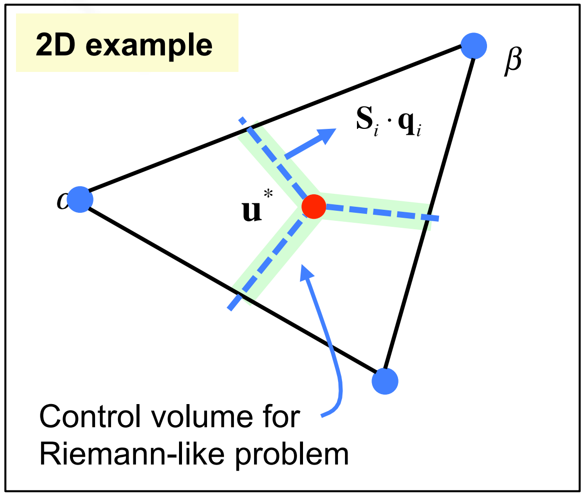
A multidirectional Riemann-like problem is solved at the center of the tetrahedron

The Riemann-like problem is based on seminal works by Despres & Mazeran (2005), Maire et. al. (2007) (2009) and Burton et. al. (2012).

Riemann force: $\mathbf{S}_i \cdot \boldsymbol{\sigma}_c^* = \mathbf{S}_i \cdot (\boldsymbol{\sigma}_c + \mathbf{q}_i)$

$$\mathbf{S}_i \cdot \mathbf{q}_i = \mu_c \left(\mathbf{u}^* - \mathbf{u}_c\right) \left|\mathbf{a}_c \cdot \mathbf{S}_i\right|$$

Momentum conservation is enforced at tetrahedron center: $\sum_{i \in \Omega_h} \mathbf{S}_i \cdot \boldsymbol{\sigma}_c^* = 0$ (13 Equations, 13 unknowns)



Riemann velocity:

$$\mathbf{u}^* = \frac{\sum_{i \in \Omega_h} \left(\mu_c \left|\mathbf{a}_c \cdot \mathbf{S}_i\right| \mathbf{u}_c - \mathbf{S}_i \cdot \boldsymbol{\sigma}_c\right)}{\sum_{i \in \Omega} \left(\mu_c \left|\mathbf{a}_c \cdot \mathbf{S}_i\right|\right)}$$

Riemann force:

$$\mathbf{S}_i \cdot \boldsymbol{\sigma}^* = \mathbf{S}_i \cdot \boldsymbol{\sigma}_c + \mu_c \left(\mathbf{u}^* - \mathbf{u}_c\right) \left|\mathbf{a}_c \cdot \mathbf{S}_i\right|$$

This Riemann-like problem was successfully applied to contact surfaces (Morgan *et. al*. JCP 2013) and SGH (Morgan *et. al*. JCP 2014).

For ALE, the mesh velocity is smoothed by solving a Laplacian equation

- The mesh velocity, **w**, dictates whether the calculation is Eulerian, essentially Lagrangian, or ALE
  - **w**=0 is the Eulerian limit
  - **w**=**u** is the essentially Lagrangian limit
  - **w**>0 and **w**<**u** is ALE
- The mesh smoothing equation (Waltz et. al. 2013) is

$$\nabla^2 \mathbf{w}_\alpha = 0$$

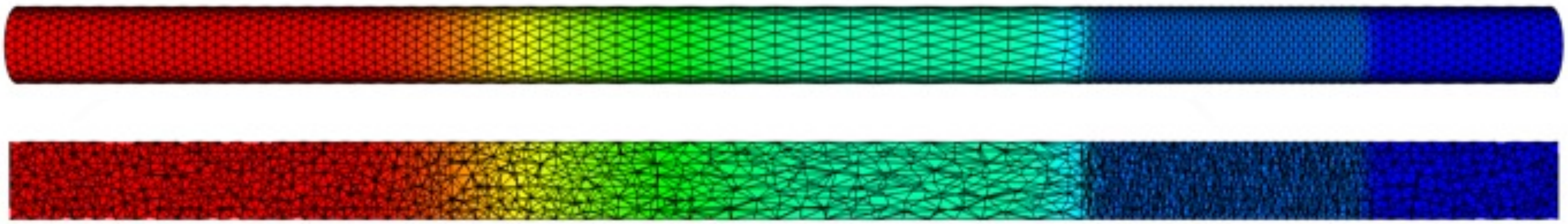
$$\mathbf{w}_\alpha^0 = \mu_\alpha \mathbf{u}_\alpha \qquad \mu_\alpha = c_1 \max\left(0, \quad 1 - c_2 \frac{\|\omega_\alpha\|}{\|\omega_\alpha\|_\infty} \right)$$

- The Laplacian is solved to a user specified tolerance

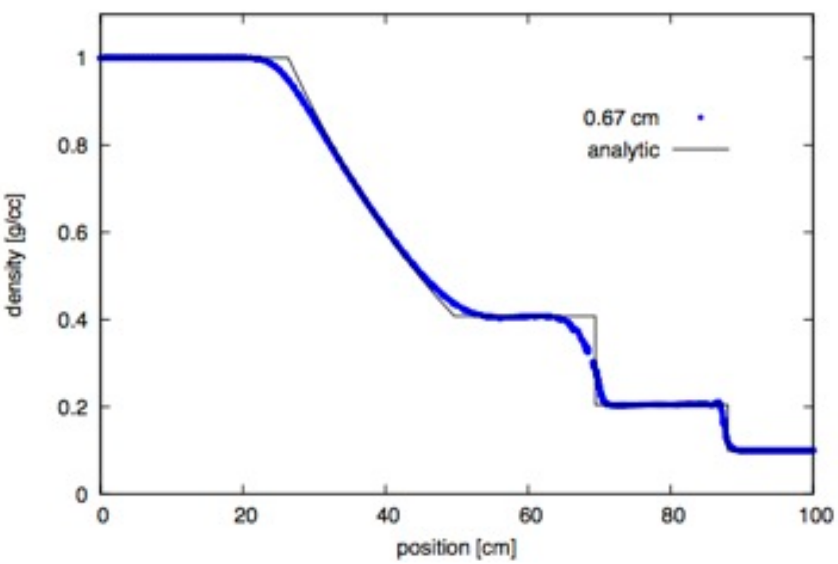
Outline

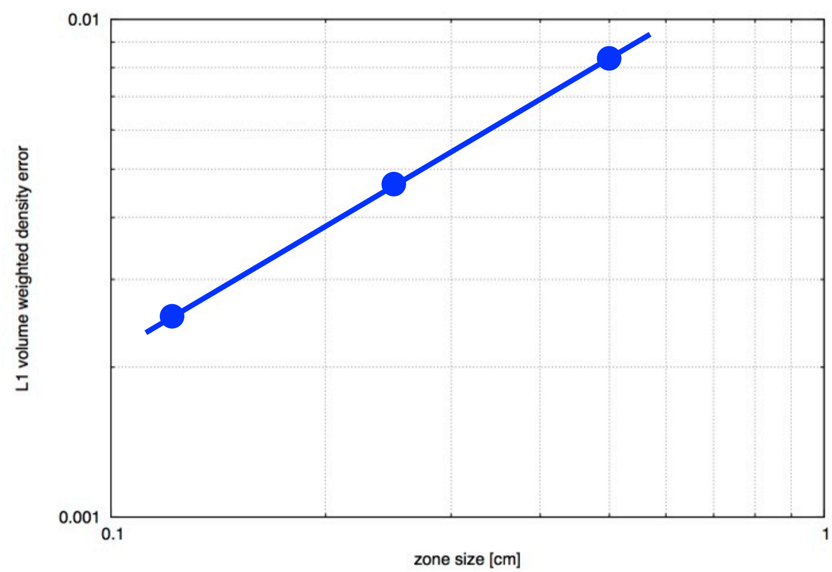
- Overview of the ALE hydrodynamic algorithm
- Lagrangian hydrodynamic test problems
- ALE hydrodynamic test problems

As demonstrated on the Sod problem, the essentially Lagrangian approach converges and is reasonably accurately on highly unstructured meshes



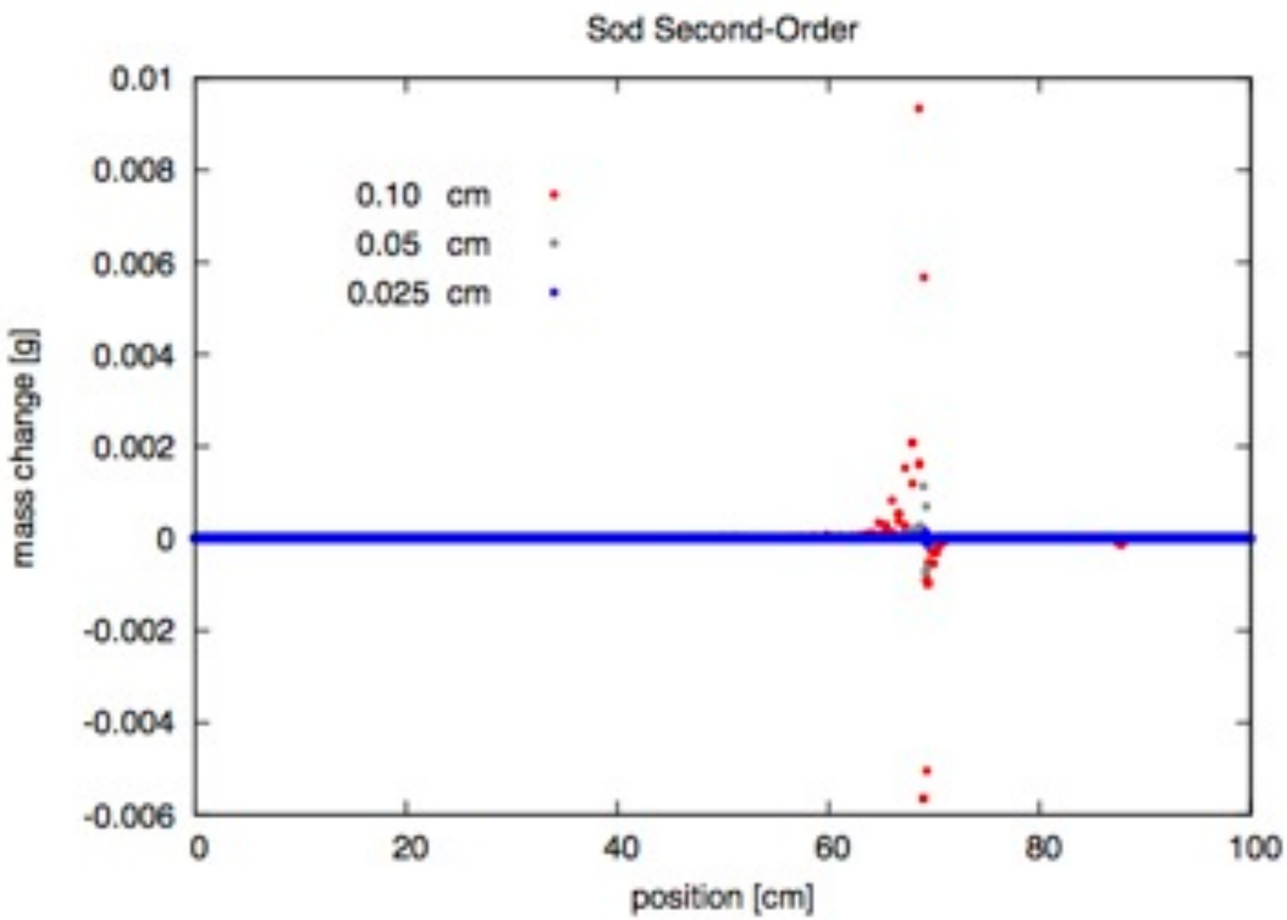
The mesh is highly irregular along the inside





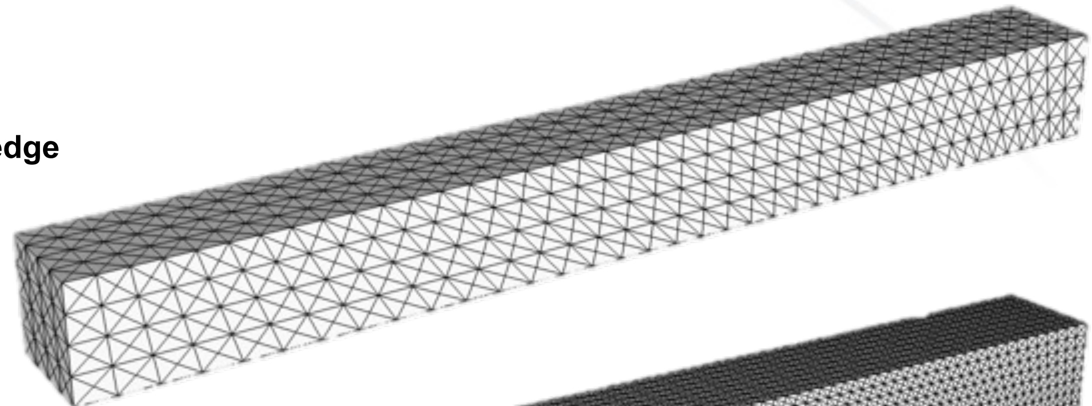
An interface treatment approach is necessary to prevent smearing of the contact discontinuity

The additional fluxes reduce to zero for smooth flows and in the limit of a zero mesh size

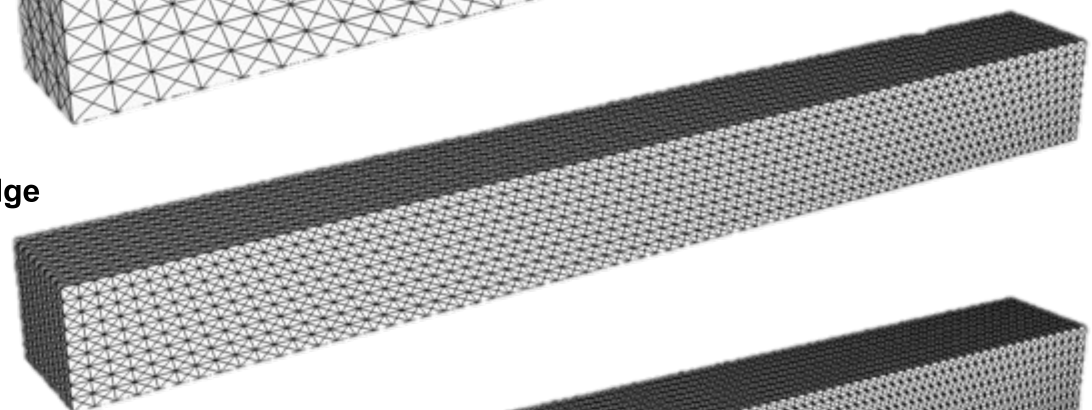


The Saltzman problem tests the robustness and symmetry preservation of a Lagrangian approach on an irregular, skewed mesh

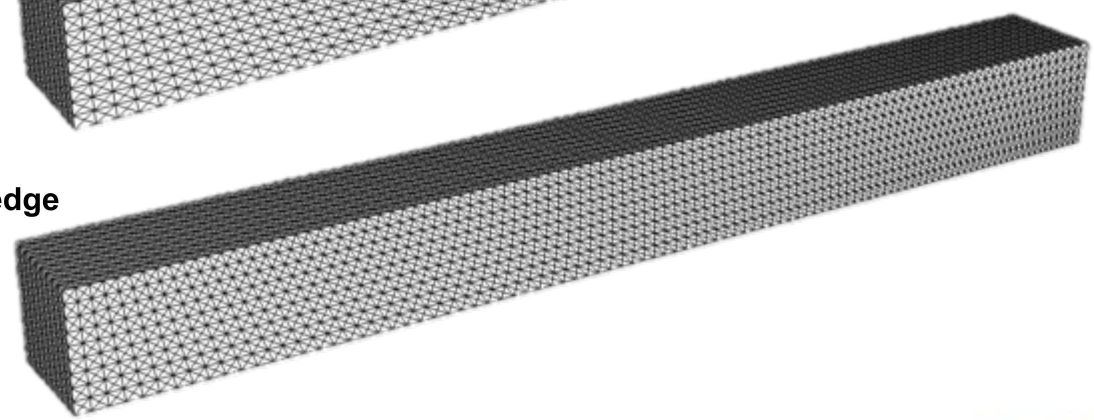
40 nodes along each edge



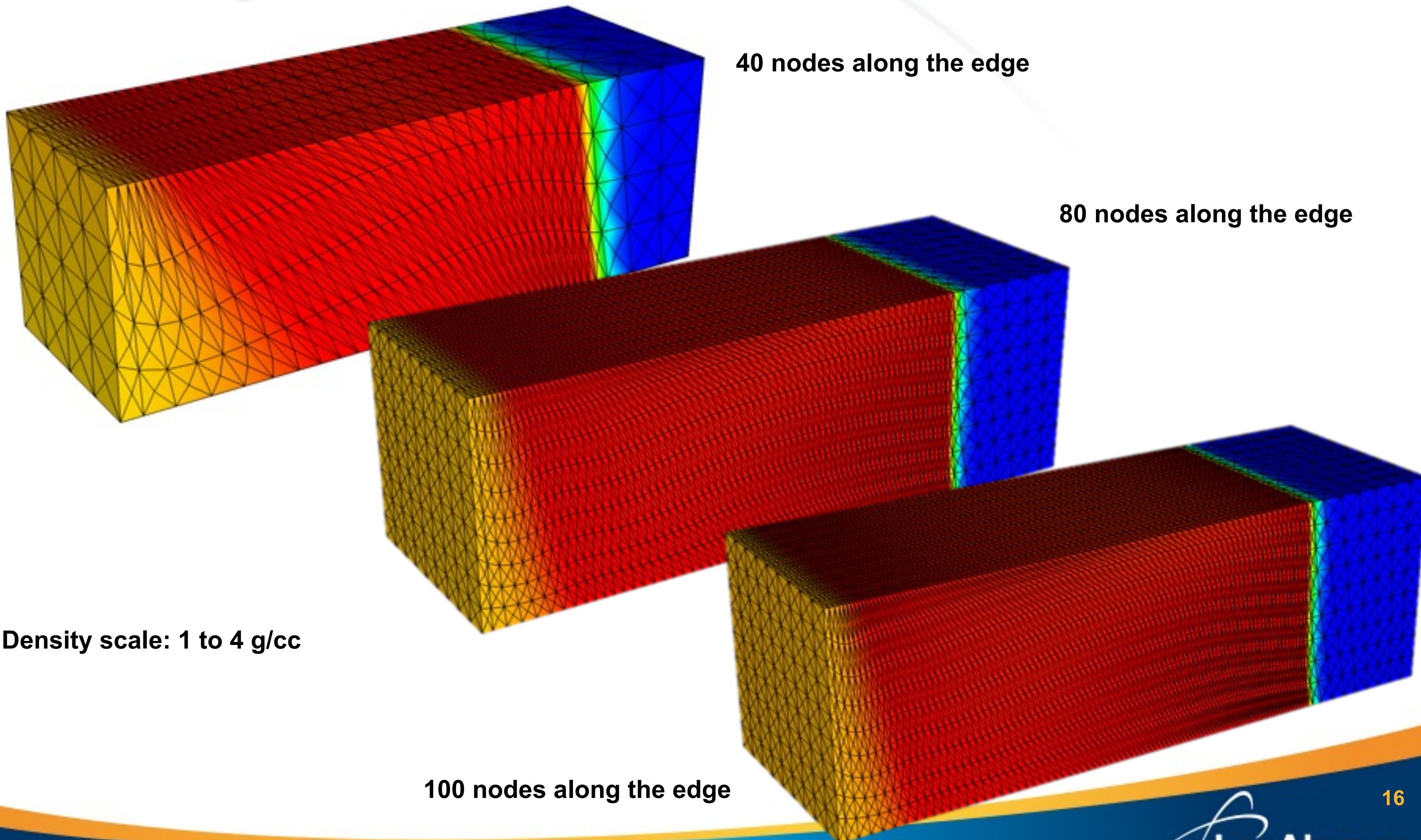
80 nodes along each edge



100 nodes along each edge



As demonstrated on Saltzman, the essentially Lagrangian approach has good mesh robustness and symmetry preservation



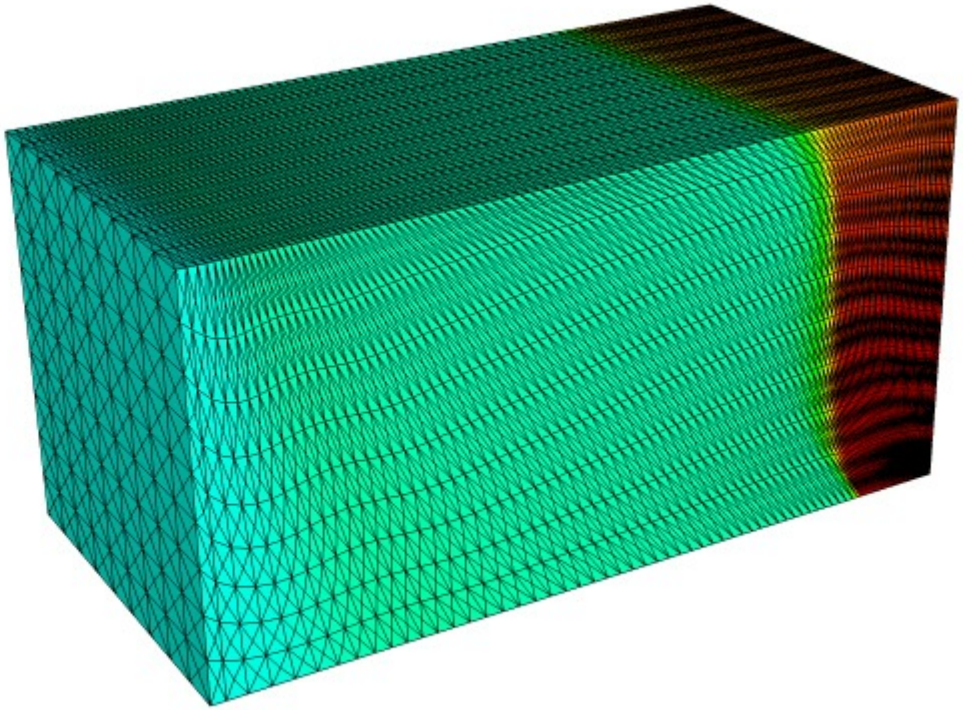
40 nodes along the edge

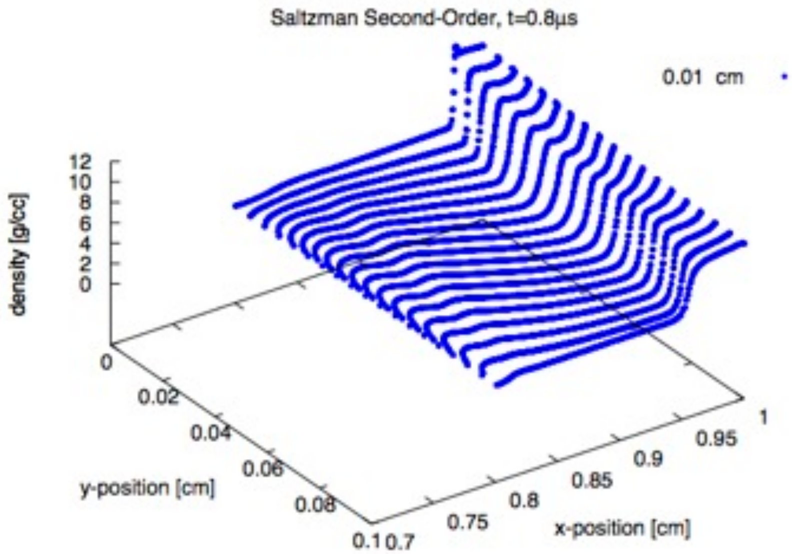
80 nodes along the edge

Density scale: 1 to 4 g/cc

100 nodes along the edge

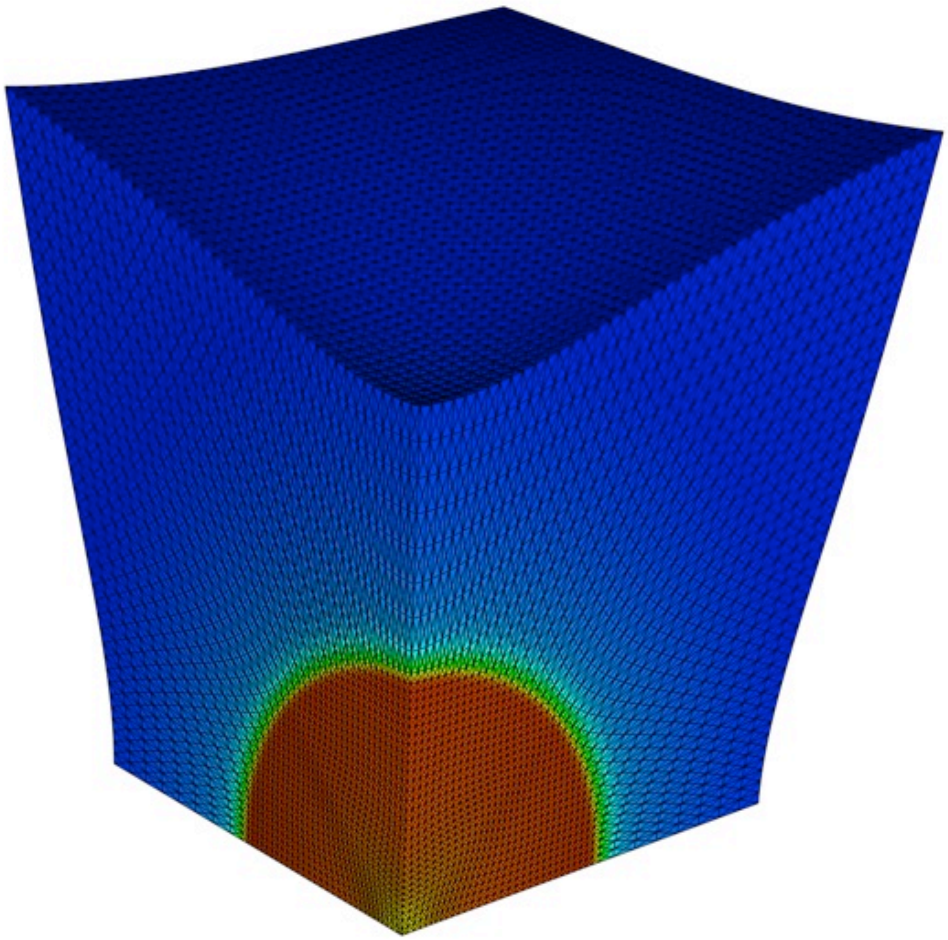
The mesh robustness on Saltzman is maintained after the shock reflects from the wall

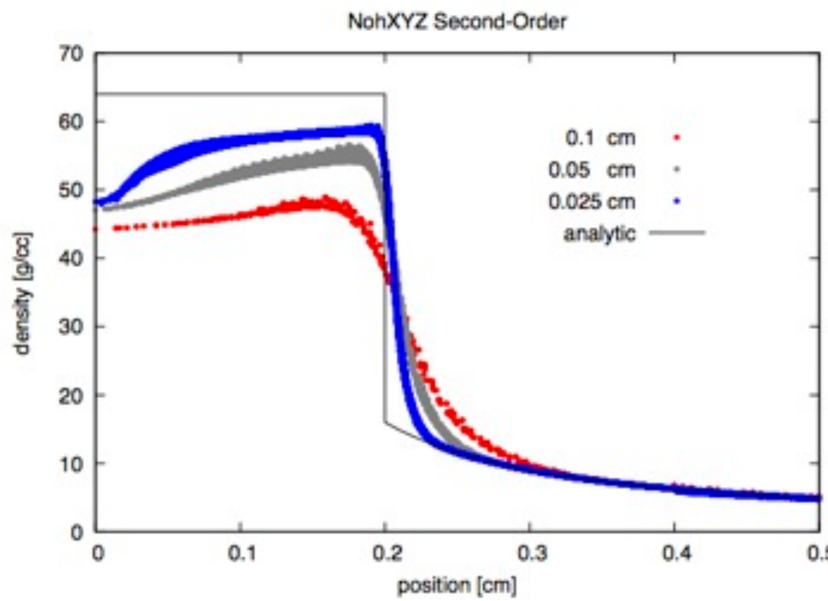




Density scale is from 1 to 10 g/cc

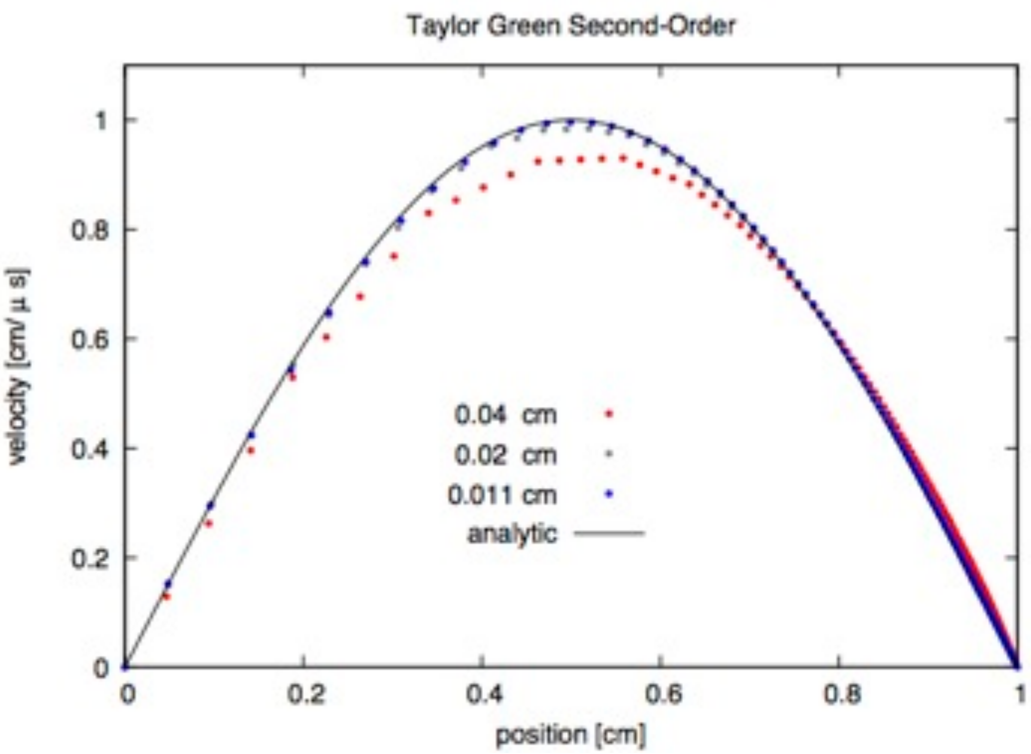
The 3D Noh problem results illustrate the essentially Lagrangian approach is accurate at converting kinetic energy into internal energy



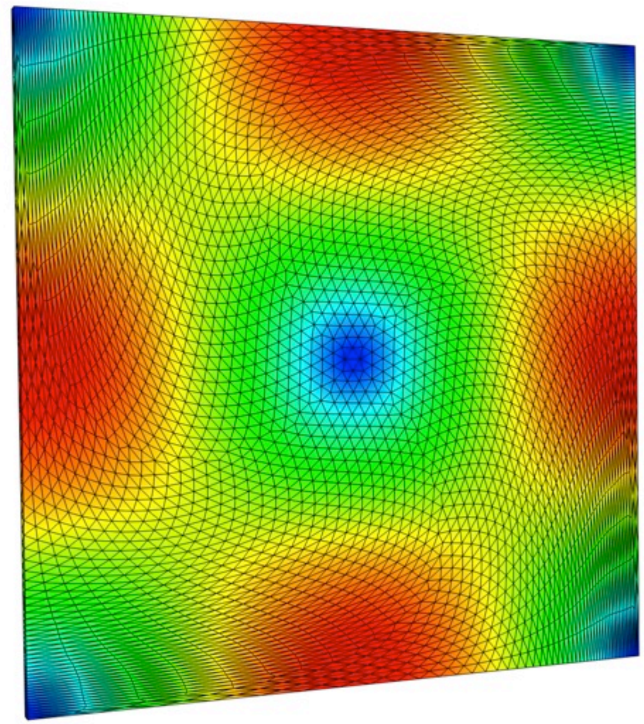


Density scale is from 2 to 64 g/cc

The Taylor Green vortex results demonstrate the essentially Lagrangian approach is accurate on a smooth flow with vorticity



T=0.5, Resolution = 0.02 cm



using a highly <u>unstructured</u> mesh

Velocity, scale 0 to 1 cm/us

Outline

- Overview of the ALE hydrodynamic algorithm
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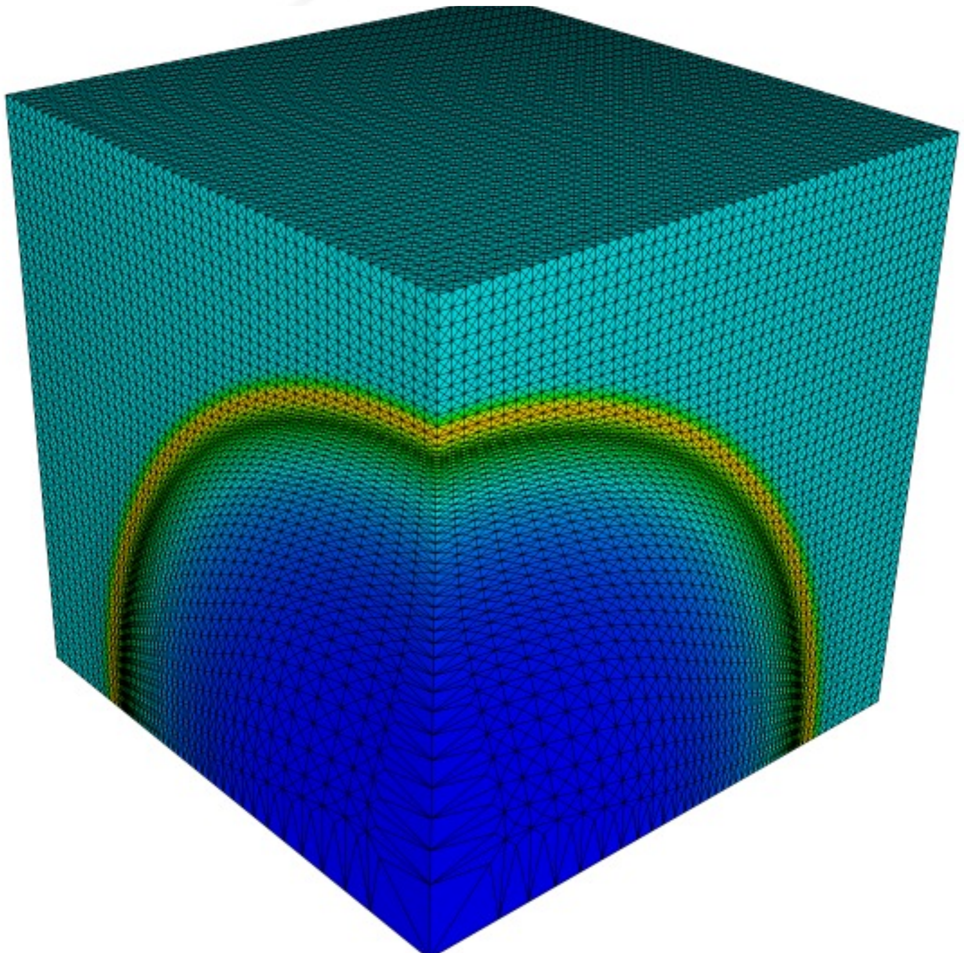
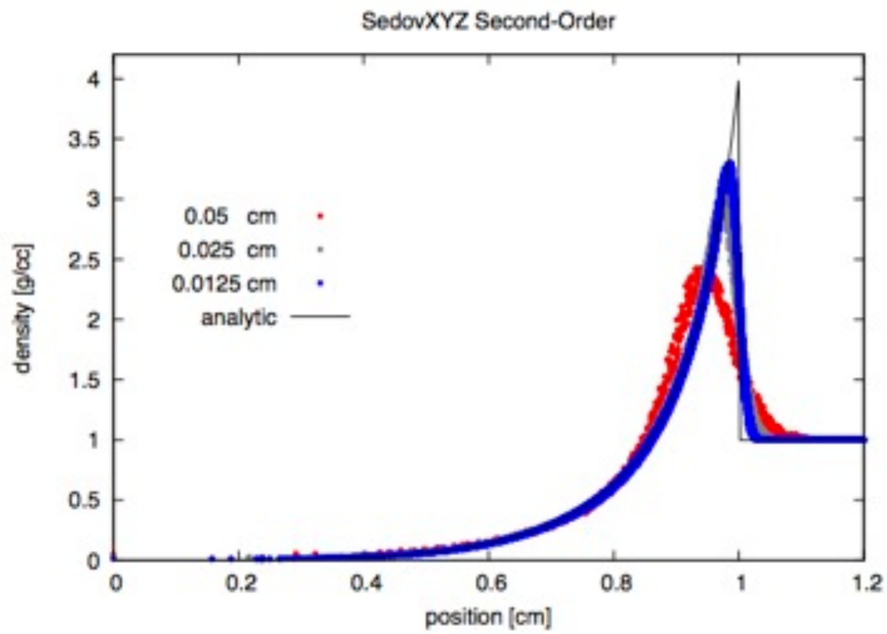
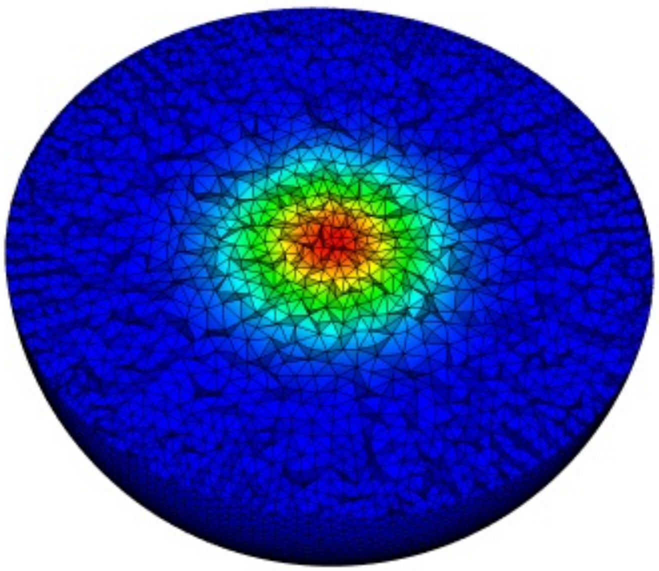
The Sedov results illustrate the new ALE approach is reasonably accurate on problems with strong shocks



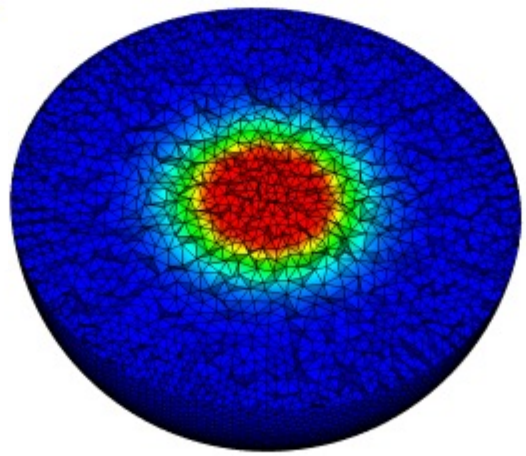


Density scale is from 0 to 4 g/cc

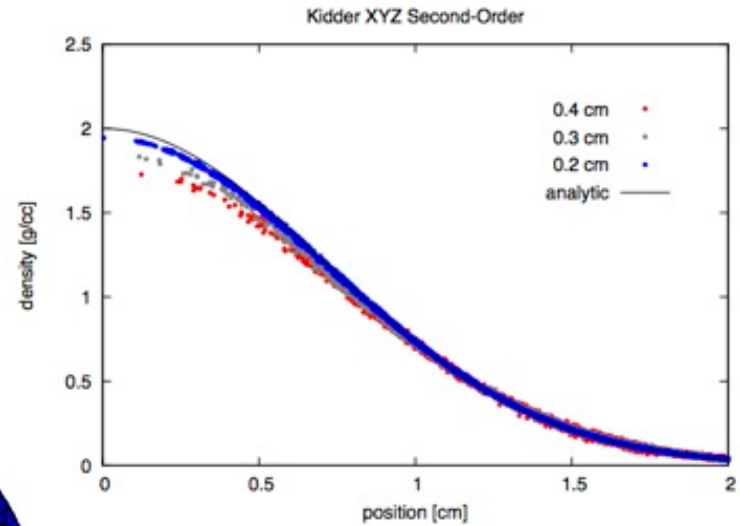
The Kidder-ball problem results demonstrate the new ALE approach is accurate on a smooth, convergent flow problem

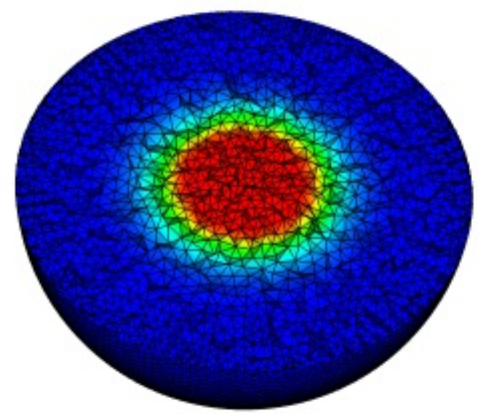


Time = 0us



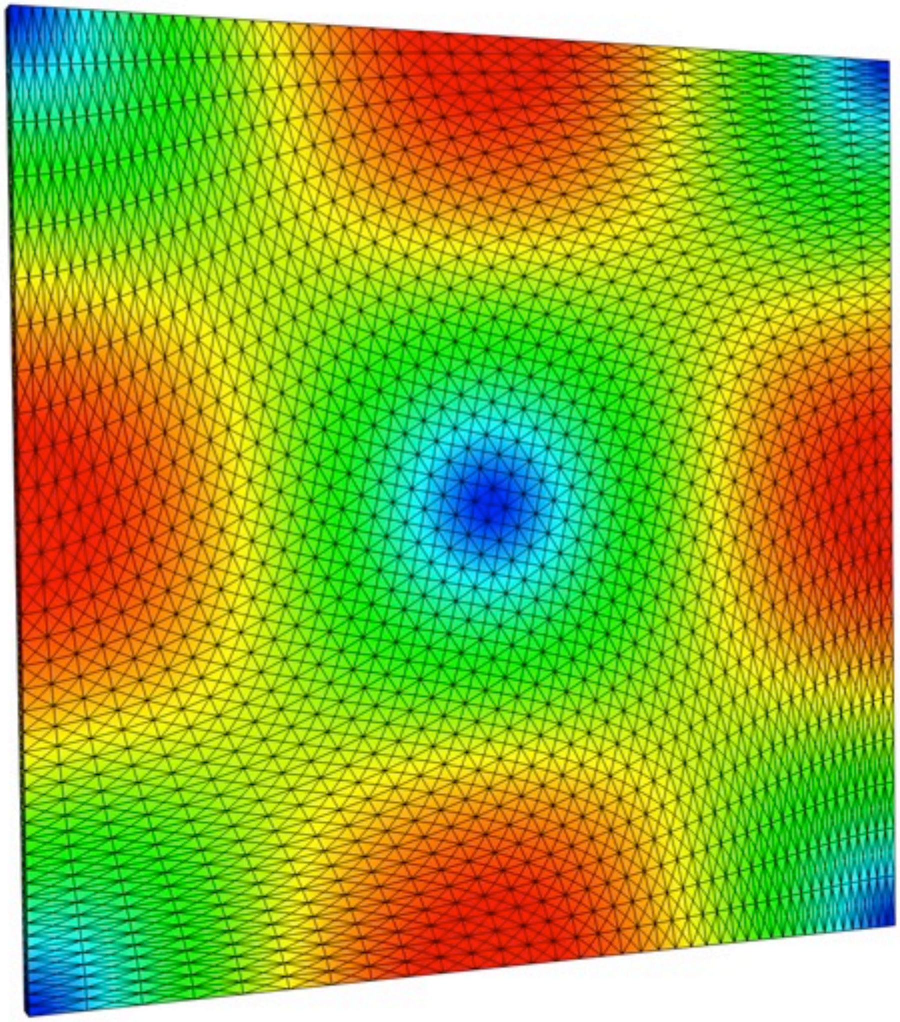
0.5us

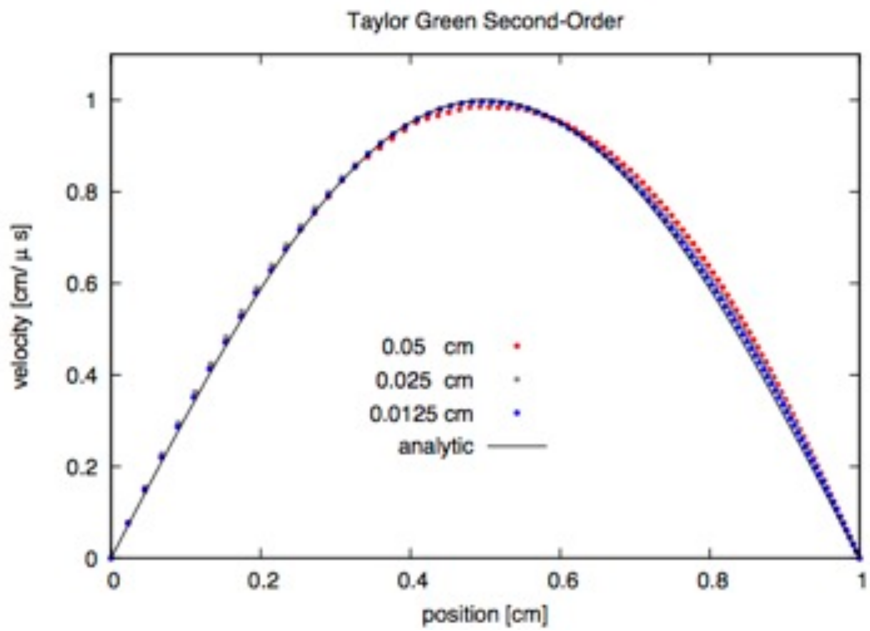




1.0us

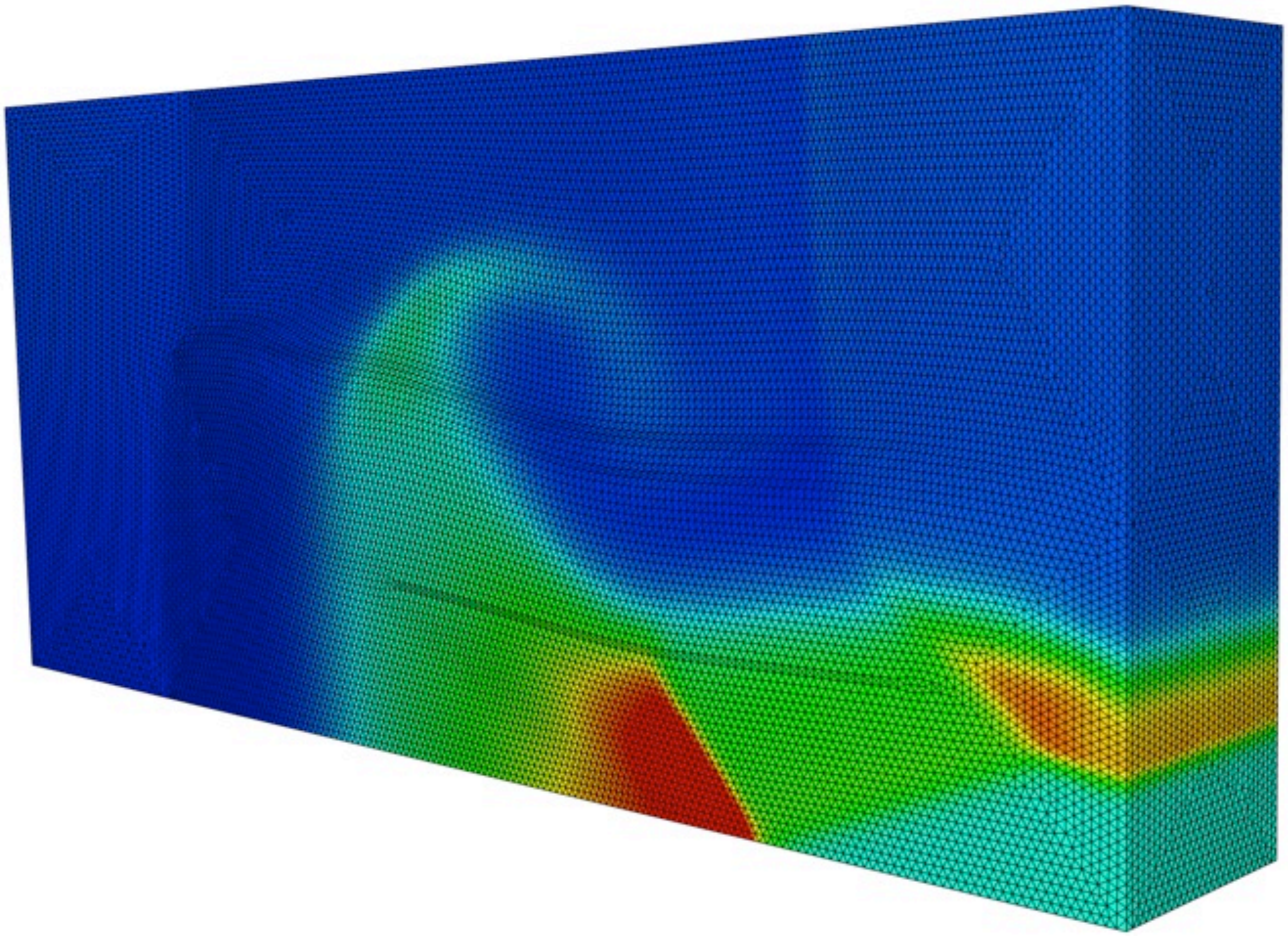
The Taylor Green vortex results illustrate the new ALE approach is accurate on smooth flow problems with physical vorticity





velocity scale is from 0 to 1 g/cc

The Triple Point problem results demonstrate the new ALE approach can model complex flows on highly unstructured meshes



density scale is from 0 to 3.5 g/cc

In conclusion

- A new ALE PCH approach was presented for modeling 3D complex flows on tetrahedral meshes
- A volume change error was discovered in Lagrangian PCH. The error arose from evolving the control volume via the average of the nodal velocities
  - The volume change error should be present in other Lagrangian methods that evolve the control volume via the average of the nodal velocities
- Additional fluxes are included to remove these volume errors
  - The fluxes go to zero in the limit of a zero mesh size or if the flow is linear
  - The fluxes must be temporally inline (Lagrange+remap will not work)
- The results from the ALE PCH approach compare favorably to analytic solutions and results from other ALE approaches
- The new approach shows promise

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