A Godunov-like point-centered ALE finite element hydrodynamic approach

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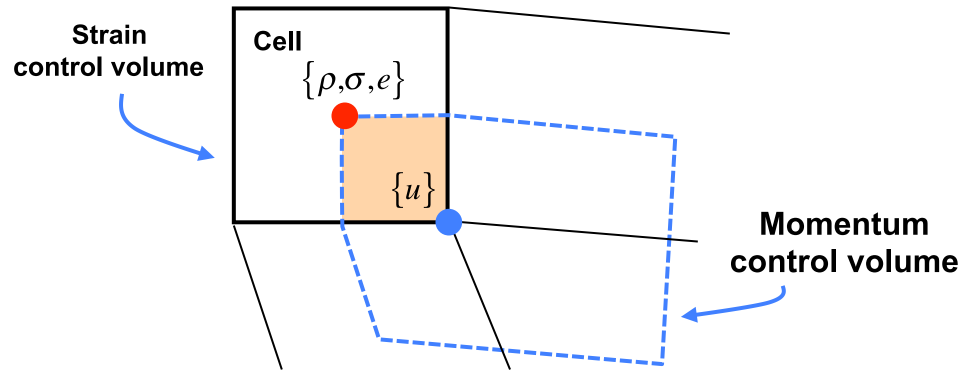
We are developing hydrodynamic methods for advanced architectures in the 3D unstructured mesh code CHICOMA

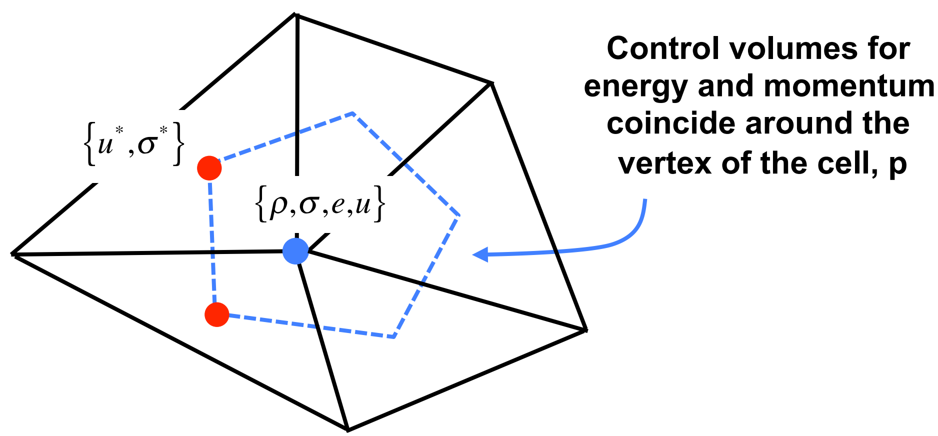
- **We seek to calculate complex 3D hydrodynamic problems**
- **These problems will require the following capabilities:**
  - **Take advantage of advanced computing architectures**
  - **Computationally more efficient than commonly used hydro codes**
  - **Simplified problem setup with commodity tools**
  - **Automatic mesh refinement (AMR) and mesh coarsening**
  - **Multiple materials**
  - **Strength**
  - **Failure**
  - **High explosives**
  - **Eulerian, Lagrangian, and ALE hydro methods**
- **Tetrahedron meshes are an option to meet these code capabilities**

Lagrangian schemes use control volumes to enforce conservation

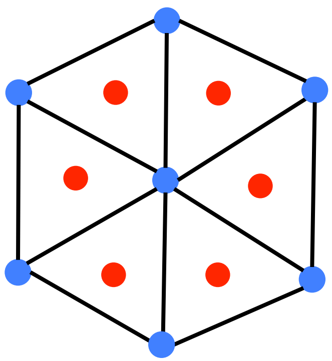
- **Staggered grid (SGH)**
  - Momentum control volume (CV) is staggered with respect to the strain/ energy volumes



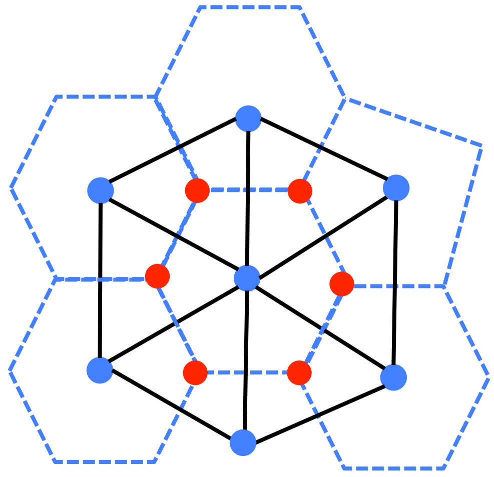
- **Point-centered (PCH) – "NEW METHOD"**
  - Control volumes coincide



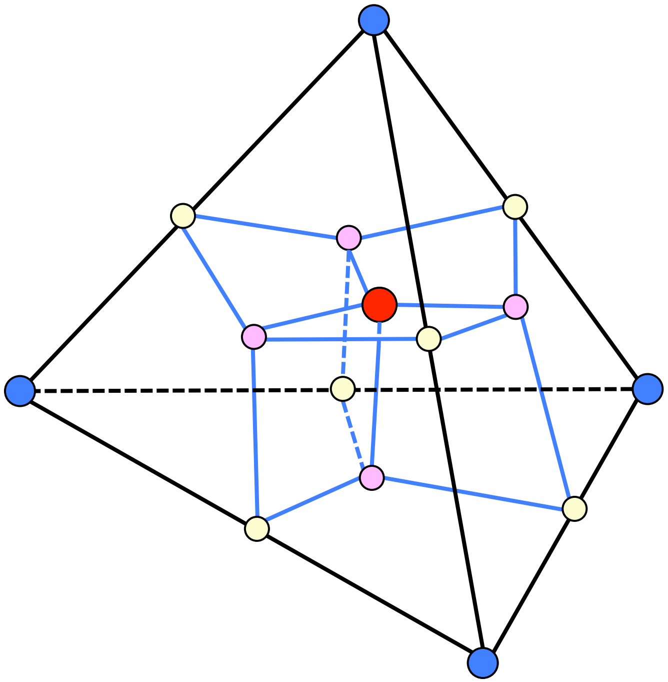
Why PCH? A PCH scheme can accurately calculate dilatation and bending on triangular or tetrahedral meshes (i.e. not stiff)



Mesh generator



Build control volumes

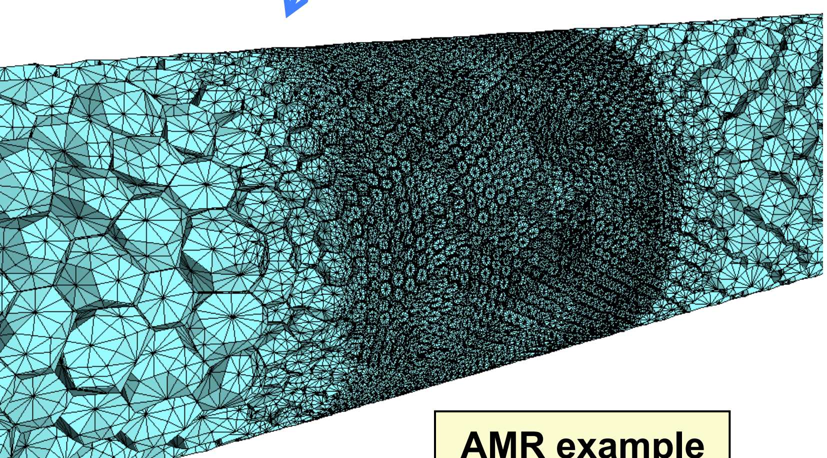


2D example

3D example

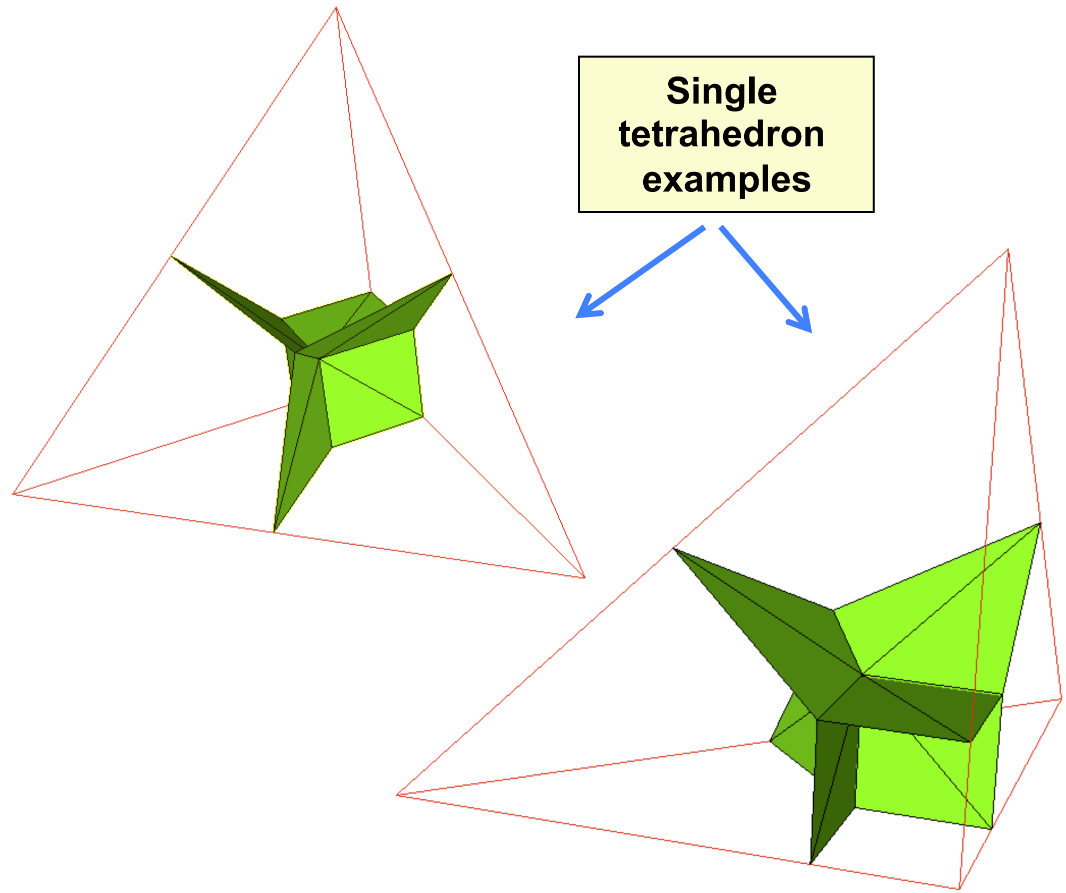
The PCH approach solves the hydrodynamic equations on arbitrary polygonal control volumes around the point

The PCH control volumes can have a large number of vertices



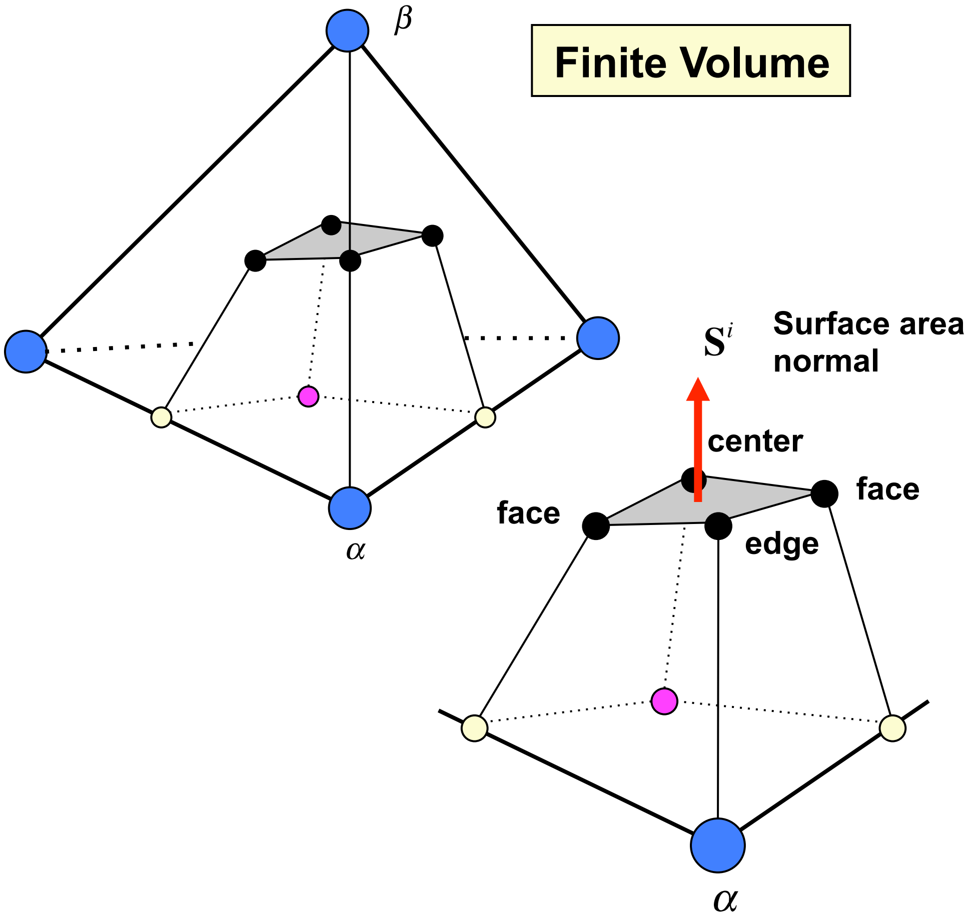
AMR example

Single tetrahedron examples

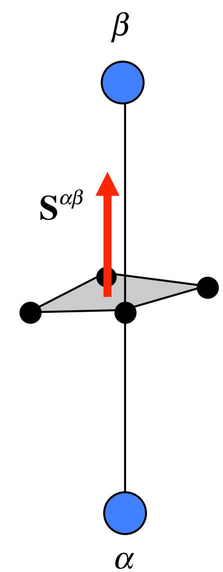


The finite element (FE) PCH approach obviates the need to explicitly calculate the control volume surfaces around the point

Finite Volume



Finite Element



Surface area normal

$$\mathbf{S}^{\alpha\beta} = \int_{\Omega_h} \left(N^\alpha \nabla N^\beta - N^\beta \nabla N^\alpha \right) d\Omega_h$$

N **= linear shape functions**

$$\mathbf{u}(x) = \sum_{\beta \in \Omega_h} N^\beta(x) \mathbf{u}^\beta$$

Important Identities:

$$\sum_{\alpha\beta \in \alpha} \mathbf{S}^{\alpha\beta} = 0$$

Closed contour around internal node α

$$\mathbf{S}^{\alpha\beta} = -\mathbf{S}^{\beta\alpha}$$

Equal and opposite on the edge between nodes α and β

$$\sum_{\alpha\beta \in \Omega_h} \mathbf{S}^{\alpha\beta} = 0$$

Equal and opposite in a tetrahedron

The discrete conservation equations for FE ALE PCH are expressed in terms of the FE surface area normal vector

Fluxes are solved in-line rather than a Lagrange + remap approach

Mass

$$\frac{\Delta M_L^\alpha}{\Delta t} = \sum_{\Omega_h \in \alpha} \sum_{\beta \in \Omega_h} \rho^{c(\alpha\beta)} \left[\mathbf{S}^{\alpha\beta} \cdot \left(\mathbf{w}^{\alpha\beta} - \mathbf{u}^* \right) \right]$$

Momentum

$$\frac{\Delta M_L^\alpha \mathbf{u}^\alpha}{\Delta t} = \sum_{\Omega_h \in \alpha} \sum_{\beta \in \Omega_h} \left(1 - \delta_{\alpha\beta}\right) \left(\mathbf{S}^{\alpha\beta} \cdot \boldsymbol{\sigma}^* \right) + \rho^{c(\alpha\beta)} \mathbf{u}^{c(\alpha\beta)} \left[\mathbf{S}^{\alpha\beta} \cdot \left(\mathbf{w}^{\alpha\beta} - \mathbf{u}^* \right) \right]$$

Total Energy

$$\frac{\Delta M_L^\alpha j^\alpha}{\Delta t} = \sum_{\Omega_h \in \alpha} \sum_{\beta \in \Omega_h} \left(1 - \delta_{\alpha\beta}\right) \left(\mathbf{S}^{\alpha\beta} \cdot \boldsymbol{\sigma}^* \cdot \mathbf{u}^* \right) + \rho^{c(\alpha\beta)} j^{c(\alpha\beta)} \left[\mathbf{S}^{\alpha\beta} \cdot \left(\mathbf{w}^{\alpha\beta} - \mathbf{u}^* \right) \right]$$

Mesh Velocity

$$\frac{\Delta \mathbf{x}^\alpha}{\Delta t} = \left(\mathbf{w}^\alpha \right)$$

$$\boldsymbol{\sigma}^* = \boldsymbol{\sigma} + \mathbf{q}^*$$ **Riemann problem**

$$\mathbf{S}^{\alpha\beta} = \int_{\Omega_h} \left(N^\alpha \nabla N^\beta - N^\beta \nabla N^\alpha \right) d\Omega_h$$ **Surface area normal**

N **= linear shape functions**

Currently, everything is spatially 1st-order accurate

Riemann-like problem

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

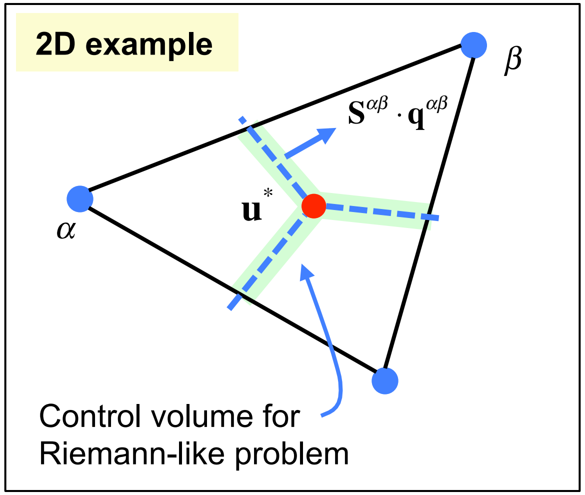
The Riemann-like problem is based on seminal works by Despres & Mazeran (2005), Maire et. al. (2007) (2009), and Burton et. al. (2012).

Riemann force: $\mathbf{S}^{\alpha\beta}\cdot\boldsymbol{\sigma}^{*} = \mathbf{S}^{\alpha\beta}\cdot\left(\boldsymbol{\sigma}^{c} + \mathbf{q}^{\alpha\beta}\right)$

Dissipation relation from Burton et. al. (2012) modified for finite element approach.

$$\mathbf{S}^{\alpha\beta}\cdot\mathbf{q}^{\alpha\beta} = \mu^{c}\left(\mathbf{u}^{*} - \mathbf{u}^{c}\right)\left|\mathbf{a}^{c}\cdot\mathbf{S}^{\alpha\beta}\right|$$

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



Riemann velocity:

$$\mathbf{u}^{*} = \frac{\sum_{\alpha\beta\in\Omega_h}\left(\mu^{c}\left|\mathbf{a}^{c}\cdot\mathbf{S}^{\alpha\beta}\right|\mathbf{u}^{c} - \mathbf{S}^{\alpha\beta}\cdot\boldsymbol{\sigma}^{c}\right)}{\sum_{\alpha\beta\in\Omega}\left(\mu^{c}\left|\mathbf{a}^{c}\cdot\mathbf{S}^{\alpha\beta}\right|\right)}$$

Riemann force:

$$\mathbf{S}^{\alpha\beta}\cdot\boldsymbol{\sigma}^{*} = \mathbf{S}^{\alpha\beta}\cdot\boldsymbol{\sigma}^{c} + \mu^{c}\left(\mathbf{u}^{*} - \mathbf{u}^{c}\right)\left|\mathbf{a}^{c}\cdot\mathbf{S}^{\alpha\beta}\right|$$

Riemann velocity and force are used in the governing equations

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

Linear projections will be used to achieve 2nd-order accuracy (work in progress)

Linear element assumption

$$\mathbf{u}(x) = \sum_{\beta \in \Omega_h} N^\beta(x)\mathbf{u}^\beta$$

Corresponding gradient for internal linear elements

$$\underbrace{\sum_{\Omega_h \in \alpha} \sum_{\beta \in \Omega_h} \int_{\Omega_h} N^\alpha N^\beta \nabla \mathbf{u}^\beta \, d\Omega_h}_{\text{Consistent mass matrix}} = \sum_{\Omega_h \in \alpha} \sum_{\beta \in \Omega_h} \mathbf{S}^{\alpha\beta}\mathbf{u}^{\alpha\beta} \longrightarrow \nabla \mathbf{u}^\alpha(x) = \frac{1}{V_L^\alpha} \sum_{\Omega_h \in \alpha} \sum_{\beta \in \Omega_h} \mathbf{S}^{\alpha\beta}\mathbf{u}^{\alpha\beta}$$

lumped mass approximation

Linear projection to center of the tetrahedron

$$\underbrace{\begin{aligned} \mathbf{u}^c &= \mathbf{u}^\beta + \mathbf{x}^{\beta k} \cdot \nabla \mathbf{u}^\beta \\ \boldsymbol{\sigma}^c &= \boldsymbol{\sigma}^\beta + \mathbf{x}^{\beta k} \cdot \nabla \boldsymbol{\sigma}^\beta \end{aligned}}_{\text{2nd order approach}}$$

Relevant Definitions:

$$\mathbf{u}^{\alpha\beta} = \frac{1}{2}\left(\mathbf{u}^\alpha + \mathbf{u}^\beta\right)$$ **value on the center of control volume face**

$$V_L^\alpha = \sum_{\Omega_h \in \alpha} \frac{1}{4}\Omega_h$$ **lumped mass**

$$\mathbf{S}^{\alpha\beta} = \int_{\Omega_h} \left(N^\alpha \nabla N^\beta - N^\beta \nabla N^\alpha\right) d\Omega_h$$ **Surface area normal**

The dissipation from the Riemann-like solver reduces to zero for a linear velocity and stress field

$$\mathbf{u}^k = \mathbf{u}^{c1} = \mathbf{u}^{c2} = \mathbf{u}^{c3} = \mathbf{u}^{c4}$$

$$\boldsymbol{\sigma}^k = \boldsymbol{\sigma}^{c1} = \boldsymbol{\sigma}^{c2} = \boldsymbol{\sigma}^{c3} = \boldsymbol{\sigma}^{c4}$$

All linear projected values from are the same in a linear field

Substitute into Riemann-like solution

$$\mathbf{u}^* = \frac{\sum_{\alpha\beta\in\Omega_h}\left(\mu^c\left|\mathbf{a}^c\cdot\mathbf{S}^{\alpha\beta}\right|\mathbf{u}^c - \mathbf{S}^{\alpha\beta}\cdot\boldsymbol{\sigma}^c\right)}{\sum_{\alpha\beta\in\Omega}\left(\mu^c\left|\mathbf{a}^c\cdot\mathbf{S}^{\alpha\beta}\right|\right)} \rightarrow \mathbf{u}^* = \mathbf{u}^k \underbrace{\cancel{\frac{\sum_{\alpha\beta\in\Omega_h}\mu^c\left|\mathbf{a}^c\cdot\mathbf{S}^{\alpha\beta}\right|}{\sum_{\alpha\beta\in\Omega}\left(\mu^c\left|\mathbf{a}^c\cdot\mathbf{S}^{\alpha\beta}\right|\right)}}}_{1} - \underbrace{\cancel{\frac{\left(\sum_{\alpha\beta\in\Omega_h}\mathbf{S}^{\alpha\beta}\right)}{\sum_{\alpha\beta\in\Omega}\left(\mu^c\left|\mathbf{a}^c\cdot\mathbf{S}^{\alpha\beta}\right|\right)}}}_{0}\cdot\boldsymbol{\sigma}^k$$

Dissipation:

$$\mathbf{S}^{\alpha\beta}\cdot\mathbf{q}^c = \mu^c\underbrace{\left(\mathbf{u}^* - \mathbf{u}^k\right)}_{=0}\left|\mathbf{a}^c\cdot\mathbf{S}^{\alpha\beta}\right|$$

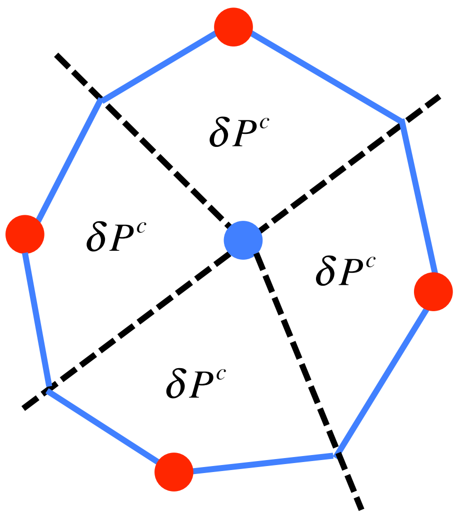
$$\mathbf{u}^* = \mathbf{u}^k$$

$$\mathbf{S}^{\alpha\beta}\cdot\boldsymbol{\sigma}^* = \mathbf{S}^{\alpha\beta}\cdot\boldsymbol{\sigma}^k$$

For a linear field and a linear projection, the Riemann values are the tetrahedron center value

The robustness of <u>pure</u> Lagrangian hydro is increased by using corner pressures calculated from the corner volumes

The approach follows the temporary quadrilateral subzoning (TQS) approach in SGH



$$P^c = P^z + \delta P^c$$

$$dP = d\rho \left.\frac{\partial p}{\partial \rho}\right|_s + \cancelto{0}{ds \left.\frac{\partial p}{\partial s}\right|_\rho}$$

Thermodynamic extrapolation along an isentrope

$$\delta P^c \approx \left(\rho^c - \rho^z\right)\left(c^z\right)^2$$

$$\delta P^c \approx \left(\frac{M^c}{V^c} - \frac{M^z}{V^z}\right)\left(c^z\right)^2$$

$$\approx \left(\frac{\left(\rho^z V^c\right)^{n=0}}{V^c} - \frac{\left(\rho^z V^z\right)^{n=0}}{V^z}\right)\left(c^z\right)^2$$

$$\approx \left(\rho^z\right)^{n=0}\left(\frac{\left(V^c\right)^{n=0}}{V^c} - \frac{\left(V^z\right)^{n=0}}{V^z}\right)\left(c^z\right)^2$$

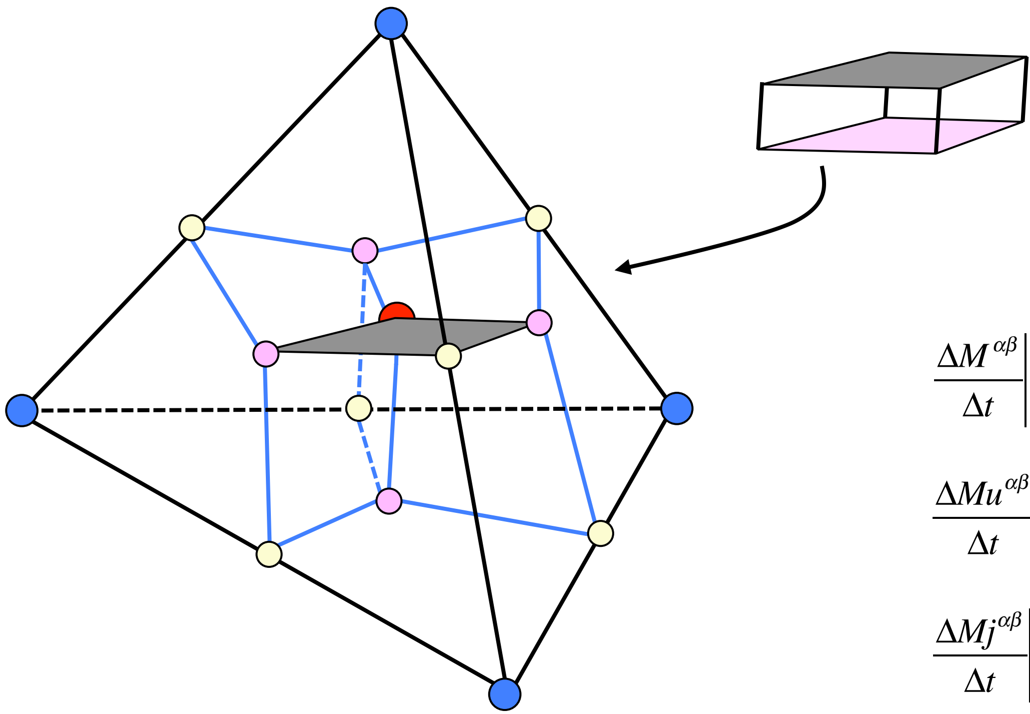
$$\boxed{\delta P^c \approx \left(\rho^z\right)^{n=0}\left(\frac{\left(V^c\right)^{n=0}}{V^c} - \frac{\left(V^z\right)^{n=0}}{V^z}\right)\left(c^z\right)^2}$$

SGH:
Burton (1992)
Caramana et. al. (1998)

Arbitrary Lagrangian Eulerian (ALE)

The fluxes are calculated similarly to traditional swept-face remap methods

Advected volume:



$$\frac{\Delta V^{flux}}{\Delta t} = \mathbf{S}^{\alpha\beta}\cdot\left(\mathbf{w}^{\alpha\beta}-\mathbf{u}^{*}\right)$$

Corner value at CV face
(per upwind stability condition)

$$\left.\frac{\Delta M^{\alpha\beta}}{\Delta t}\right|^{flux} = \rho^{c(\alpha\beta)}\left[\mathbf{S}^{\alpha\beta}\cdot\left(\mathbf{w}^{\alpha\beta}-\mathbf{u}^{*}\right)\right]$$

$$\left.\frac{\Delta M u^{\alpha\beta}}{\Delta t}\right|^{flux} = \rho^{c(\alpha\beta)}\mathbf{u}^{c(\alpha\beta)}\left[\mathbf{S}^{\alpha\beta}\cdot\left(\mathbf{w}^{\alpha\beta}-\mathbf{u}^{*}\right)\right]$$

$$\left.\frac{\Delta M j^{\alpha\beta}}{\Delta t}\right|^{flux} = \rho^{c(\alpha\beta)} j^{c(\alpha\beta)}\left[\mathbf{S}^{\alpha\beta}\cdot\left(\mathbf{w}^{\alpha\beta}-\mathbf{u}^{*}\right)\right]$$

Currently, the corner values are equal to the point values (i.e. spatially 1st-order)

Time Integration

A multistage Runge-Kutta time integration approach is used to evolve the governing equations in time

Runge-Kutta time integration

$$U^{k+1} = U^n + \theta^k RHS^k$$

$$\theta^k = \frac{1}{n_{stage} + 1 - k} \qquad \begin{cases} \theta^{k=1} = \theta^n \\ \theta^{k=n_{stage}} = \theta^{n+1} \end{cases}$$

Governing ALE equations

$$\left(M_L^{\alpha}\right)^{k+1} = \left(M_L^{\alpha}\right)^n + \theta^k \Delta t \left(\sum_{\Omega_h \in \alpha} \sum_{\beta \in \Omega_h} \rho^{c(\alpha\beta)} \left[\mathbf{S}^{\alpha\beta} \cdot \left(\mathbf{w}^{\alpha\beta} - \mathbf{u}^* \right) \right] \right)^k$$

$$\left(M_L^{\alpha} \mathbf{u}^{\alpha}\right)^{k+1} = \left(M_L^{\alpha} \mathbf{u}^{\alpha}\right)^n + \theta^k \Delta t \left(\sum_{\Omega_h \in \alpha} \sum_{\beta \in \Omega_h} \left(1 - \delta_{\alpha\beta}\right) \left(\mathbf{S}^{\alpha\beta} \cdot \boldsymbol{\sigma}^* \right) + \rho^{c(\alpha\beta)} \mathbf{u}^{c(\alpha\beta)} \left[\mathbf{S}^{\alpha\beta} \cdot \left(\mathbf{w}^{\alpha\beta} - \mathbf{u}^* \right) \right] \right)^k$$

$$\left(M_L^{\alpha} j^{\alpha}\right)^{k+1} = \left(M_L^{\alpha} j^{\alpha}\right)^n + \theta^k \Delta t \left(\sum_{\Omega_h \in \alpha} \sum_{\beta \in \Omega_h} \left(1 - \delta_{\alpha\beta}\right) \left(\mathbf{S}^{\alpha\beta} \cdot \boldsymbol{\sigma}^* \cdot \mathbf{u}^* \right) + \rho^{c(\alpha\beta)} j^{c(\alpha\beta)} \left[\mathbf{S}^{\alpha\beta} \cdot \left(\mathbf{w}^{\alpha\beta} - \mathbf{u}^* \right) \right] \right)^k$$

$$\left(\mathbf{x}^{\alpha}\right)^{k+1} = \left(\mathbf{x}^{\alpha}\right)^n + \theta^k \Delta t \left(\mathbf{w}^{\alpha}\right)^k$$

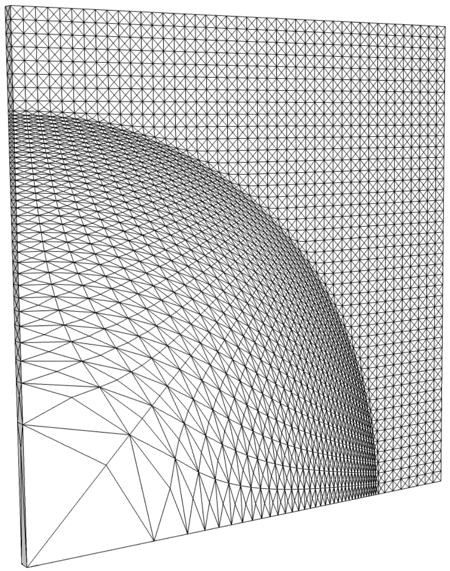
Lagrangian test problems

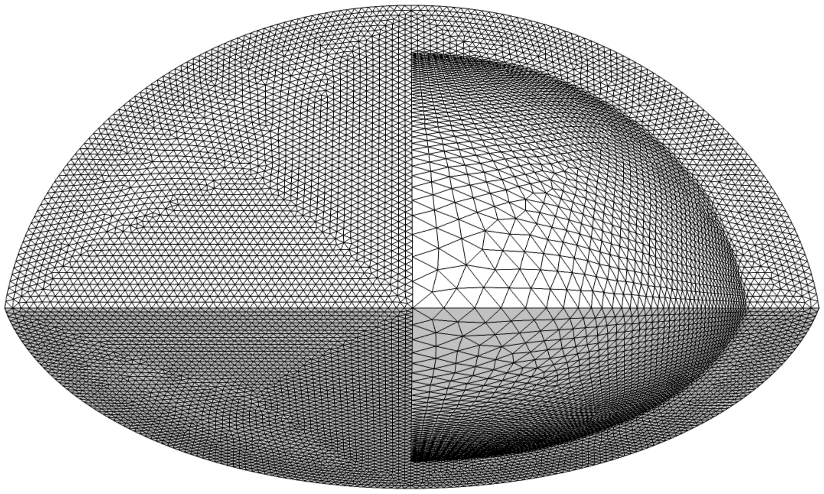
- **Fully Lagrangian (*i.e.* fluxes =0)**
- **3 stage RK time integration**
- **1st-order in space**
- **TQS**
- **Lumped mass**

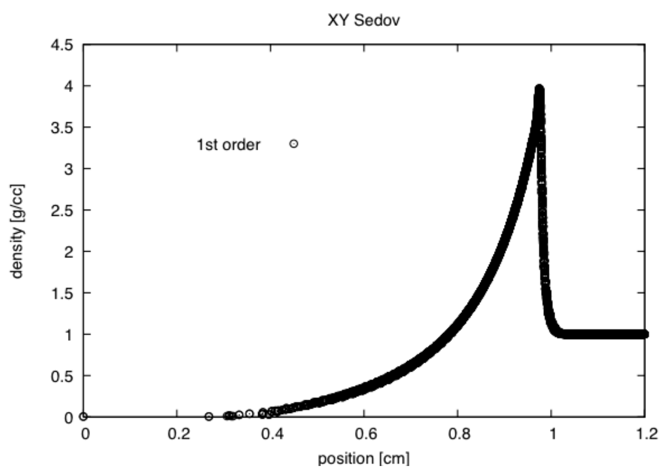
Results on Sedov indicate good mesh robustness and accuracy

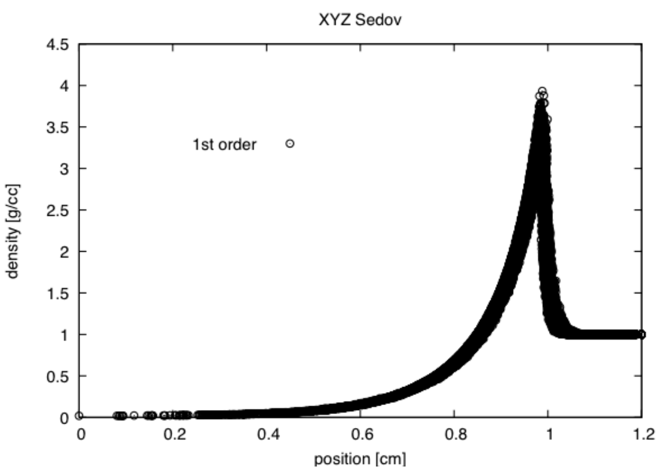
Mesh: Hexahedron cells decomposed into 24 tetrahedrons

44x44x2 nodes



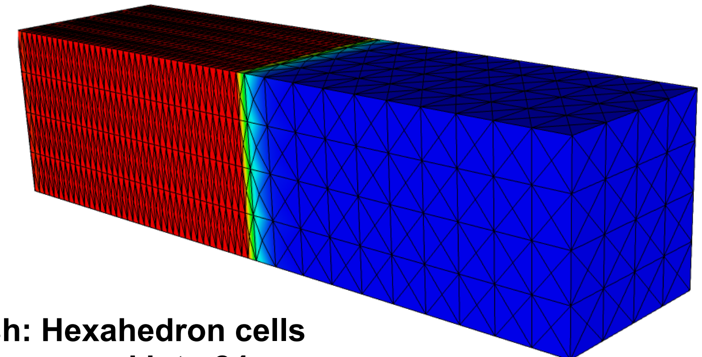




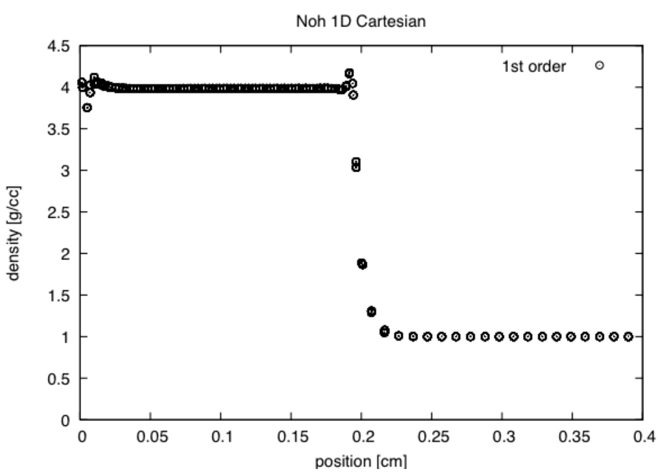


Sedov (1959)

Noh 1D Cartesian and Saltzman results demonstrate accuracy and robustness

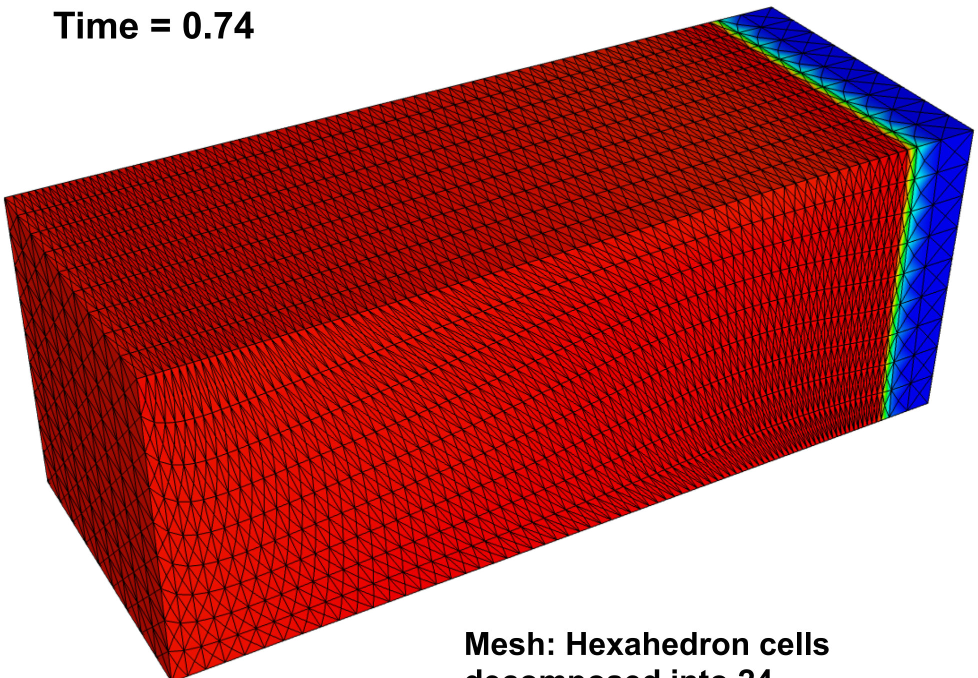


Mesh: Hexahedron cells decomposed into 24 tetrahedrons



Noh (1987)

Time = 0.74



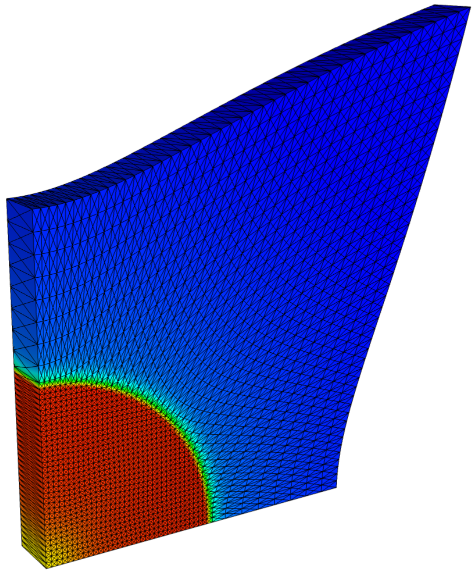
Mesh: Hexahedron cells decomposed into 24 tetrahedrons

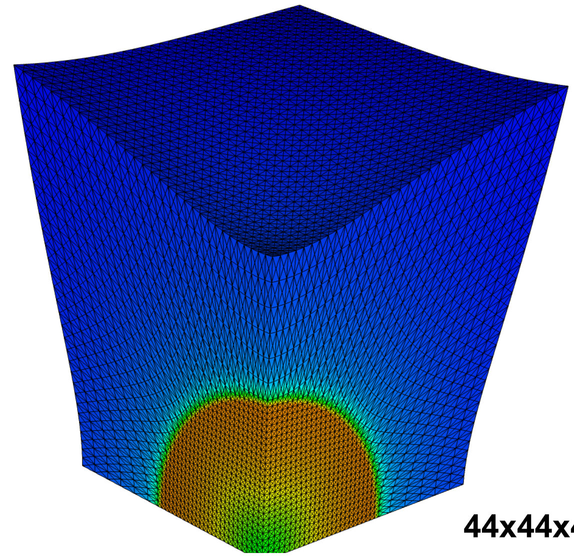
Saltzman

The Noh results demonstrate accuracy and good mesh robustness

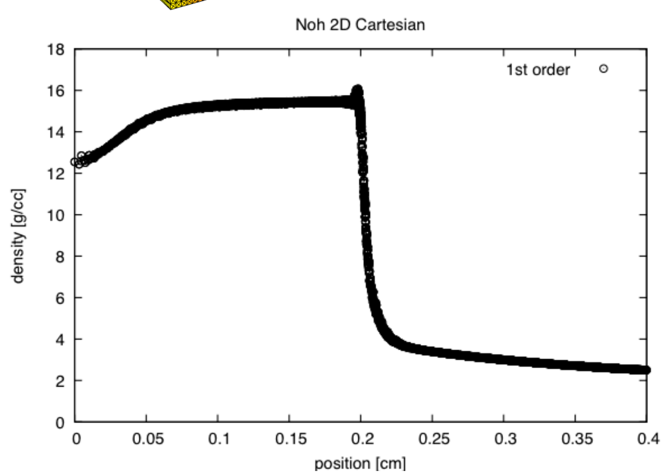
Mesh: Hexahedron cells decomposed into 24 tetrahedrons

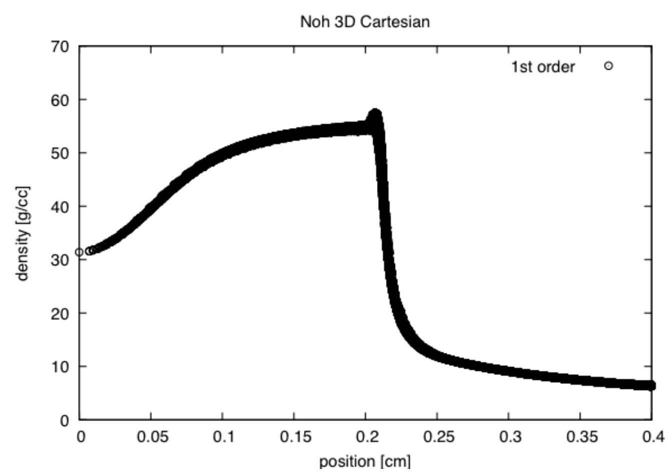
44x44x2 nodes





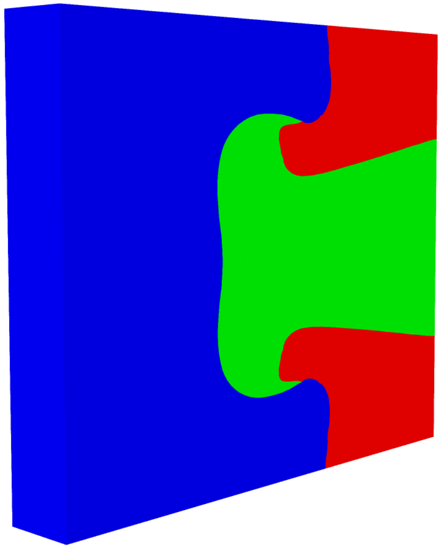
44x44x44 nodes

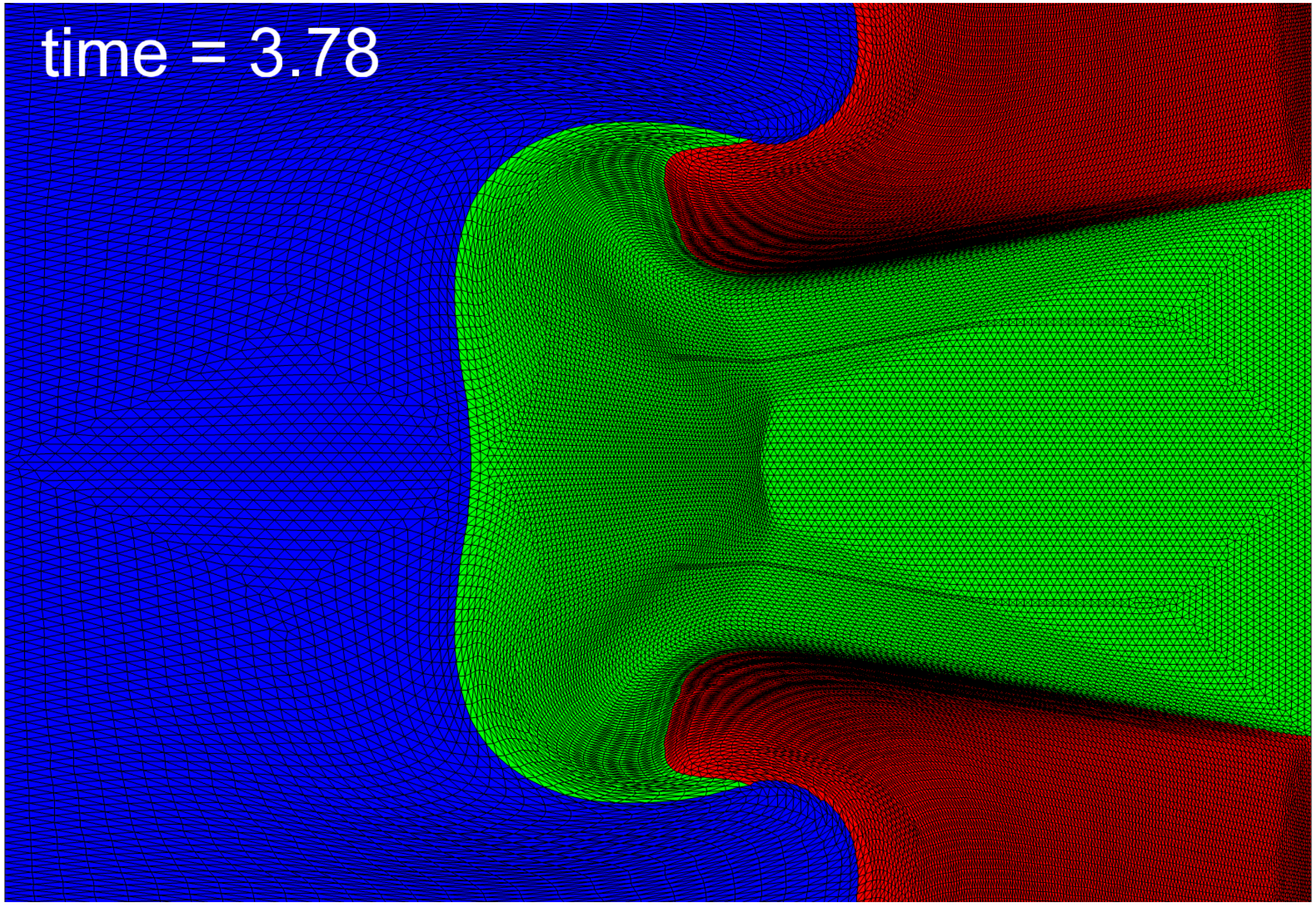




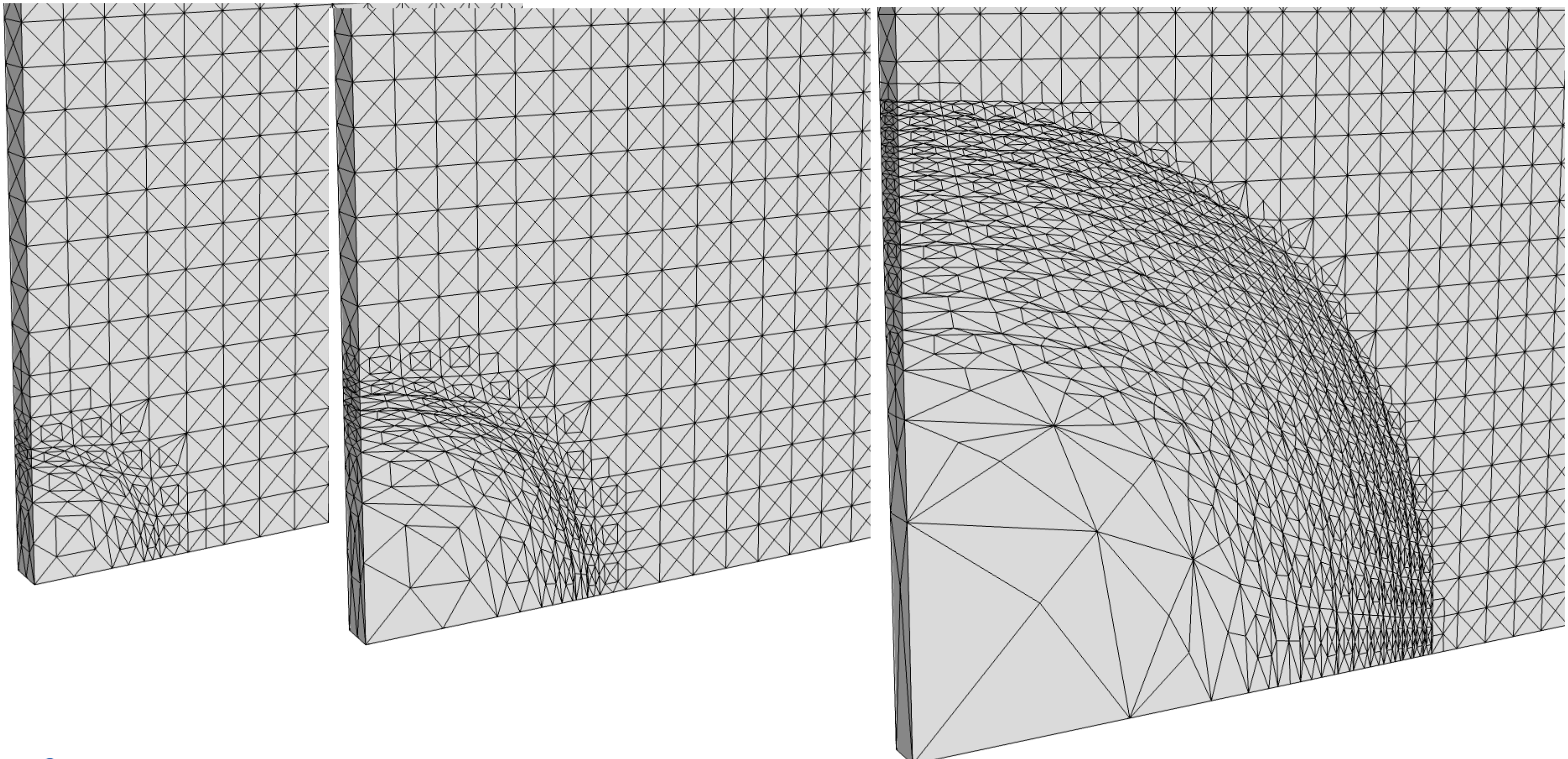
Noh (1987)

The triple point results shows excellent mesh robustness with a fully 3D unstructured Cubit mesh





Lagrangian AMR used on Sedov XY problem illustrates an advantage of a tetrahedron mesh

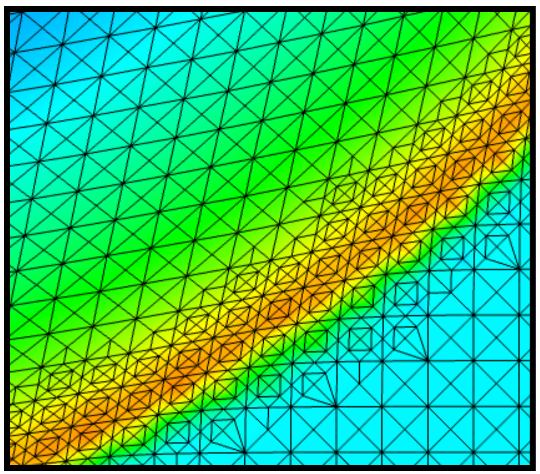


ALE test problems

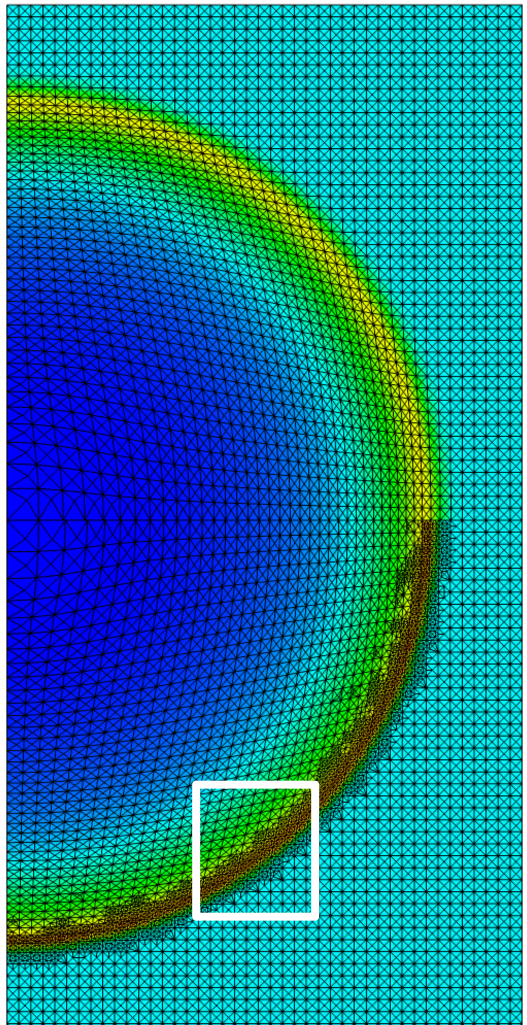
- ALE
  - Laplacian smoother applied to velocity
  - see Waltz et. al. 2013 multiMat talk
- 3-stage RK time integration
- 1st-order in space
- Lumped mass
- With and without AMR

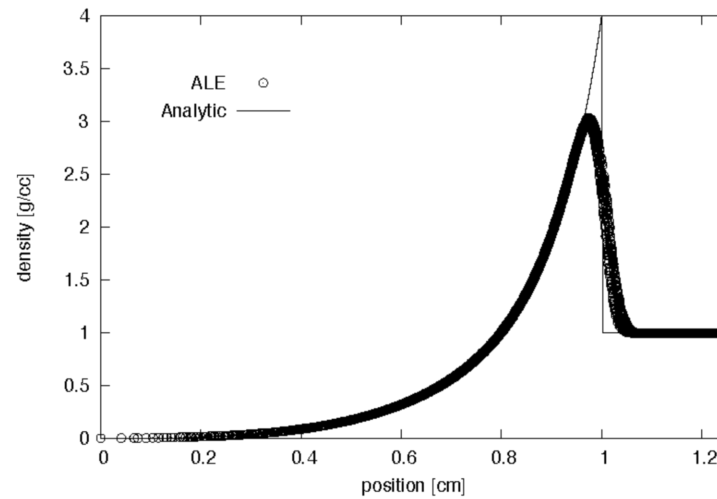
Sedov XY with ALE + AMR increases the peak density relative to the ALE calculation

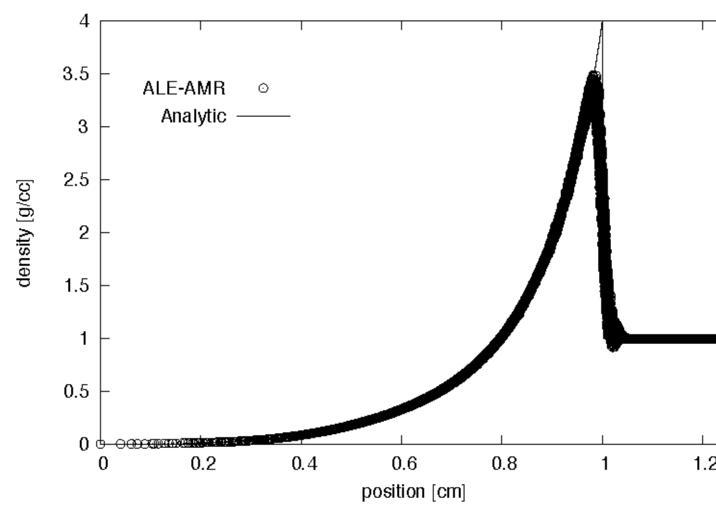
Mesh refinement and coarsening based on density gradient



Zoom

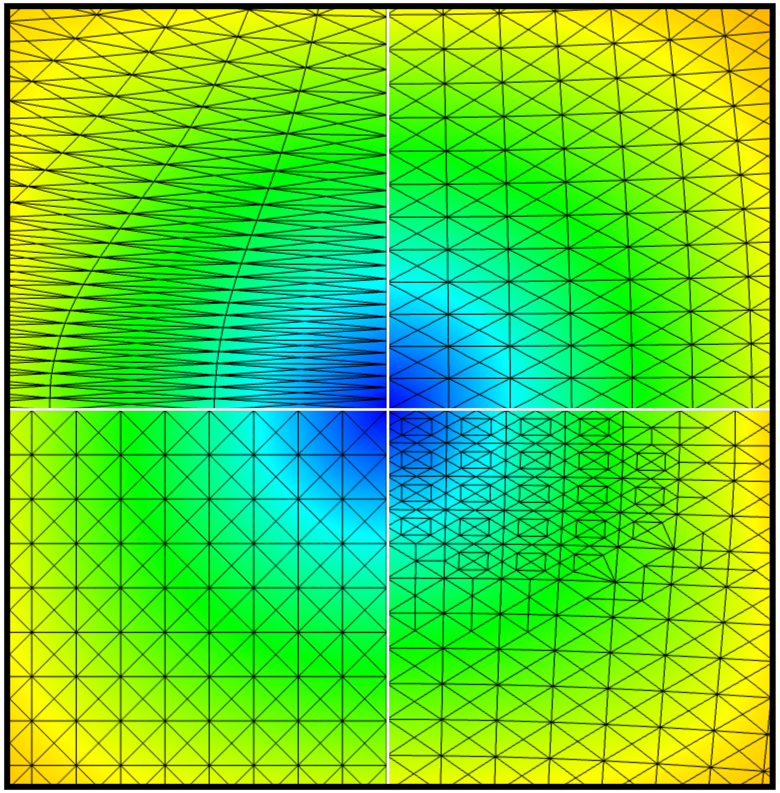






ALE+AMR is intended to improve accuracy on problems with vorticity such as the Taylor Green problem

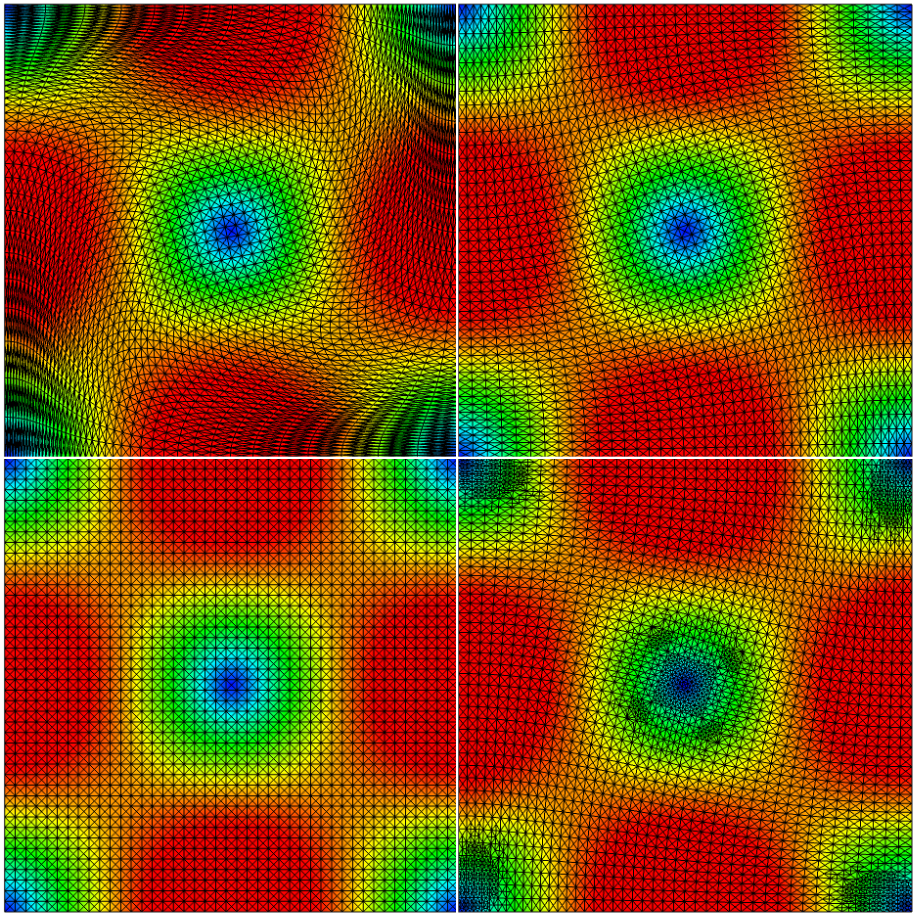
Mesh refinement and coarsening based on velocity gradient



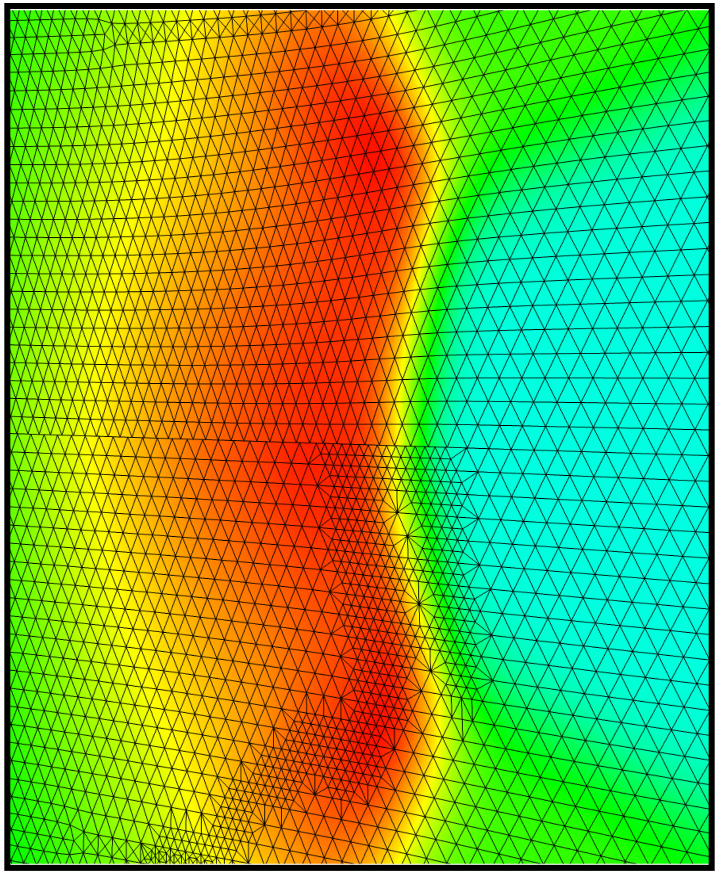
Zoom of corner

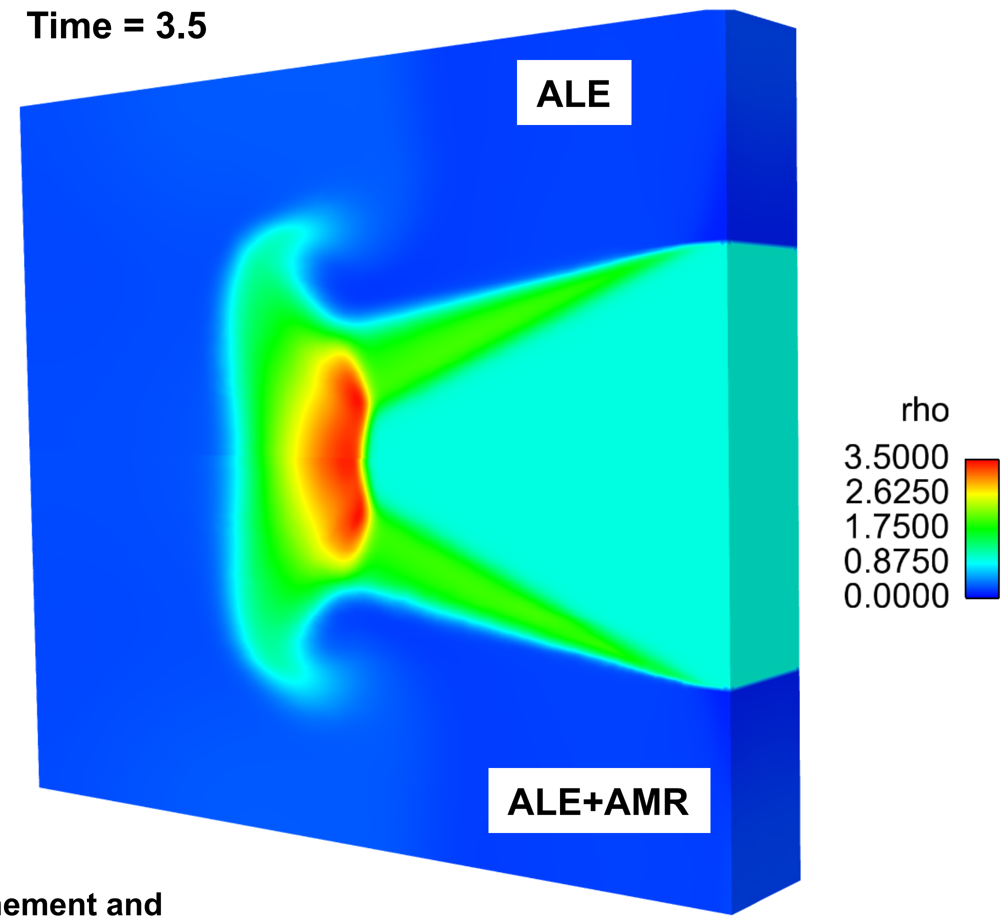
Velocity plot

Time=0.5



ALE+AMR is intended to improve accuracy on problems with vorticity such as the triple point problem





Mesh refinement and coarsening based on density gradient

Conclusion

- **Progress made on developing a PCH algorithm for tetrahedron meshes**
  - **Finite Element**
  - **ALE**
  - **Multidirectional Riemann-like problem**
  - **AMR**
- **Preliminary results (11-months into project) are encouraging**
- **Future work includes:**
  - **Improve solution at discontinuities by eliminating oscillations**
  - **Extend the algorithm to 2nd-order spatial accuracy**
  - **Research automatic mesh refinement and coarsening criteria suitable for ALE calculations**
  - **Explore velocity smoothing algorithms suitable for in-line advection**

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