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A 3D Finite Element ALE Method using an Approximate Riemann Solution

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Abstract

Finite element methods have been widely used to study the hydrodynamics of compressible flows involving strong shocks in the arbitrary Lagrangian Eulerian (ALE) framework. Recently Lagrangian methods have been proposed that solve a multidimensional Riemann-like problem at the cell center in a staggered grid hydrodynamic (SGH) arrangement. Our work builds upon and improves an earlier Lagrangian code called Cercion-3D by implementing a multidimensional Riemann-like solution for finite element SGH. In addition we extend to three dimensions a mesh relaxation and remapping technique developed in 2012. Our ALE scheme uses a compatible discretization that ensures conservation of total energy.

A test suite of three dimensional problems is explored to evaluate the fidelity of the numerical techniques in our improved Cercion-3D, including the Sedov, Noh, Verney collapsing shell, and Sod problems. We compare the analytic solutions for these problems to our calculated results using both pure Lagrangian and ALE approaches. To further evaluate our remapping technique we consider the steady state Taylor-Green vortex problem and show that our method using an approximate Riemann-like solution does not generate excessive dissipation and is able to preserve the initial velocity magnitude on an Eulerian mesh. Finally we explore the triple point problem involving a contact discontinuity and a strong shock, conditions that generate a large amount of shear-driven vorticity. We compare the amount of roll-up at the triple point with our finite element SGH method to that produced by two other higher order multi-material advection techniques.

Outline

- Elements of the Cercion 3D code
  - Finite element formulation
  - Multi-dimensional Riemann solution
  - Total energy conserving remap
- Lagrangian Test Problems
  - Sod
  - 3D Sedov
  - 3D Noh
  - Verney imploding shell
- ALE Test Problems
  - Sod
  - 3D Sedov
  - 3D Noh
  - Taylor Green Vortex
  - Triple Point
- Conclusions

The Lagrangian finite element formulation builds on the compatible finite volume approach of Burton (1994) and Caramana et. al. (1998)

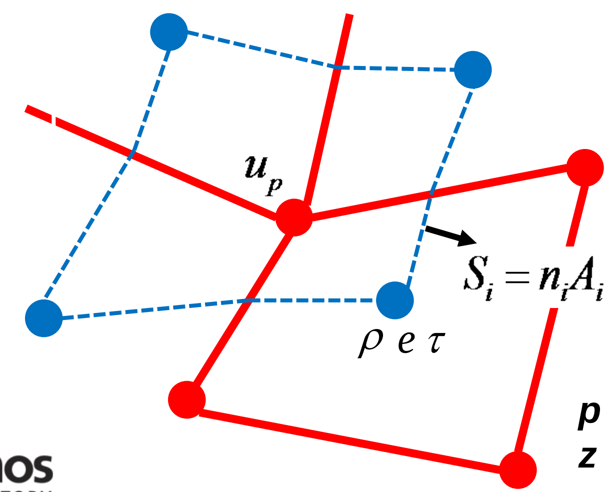
Compatible formulation of the semi-discrete Lagrangian Equations

$$M_p \frac{\Delta u}{\Delta t} = \sum_{i \in p} f_i^{n+\frac{1}{2}}$$

$$\frac{\Delta x_p}{\Delta t} = u_p^{n+\frac{1}{2}}$$

$$M_z \frac{\Delta e_z}{\Delta t} = -\sum_{i \in z} \left(f_i^{n+\frac{1}{2}} \bullet u_p^{n+\frac{1}{2}} \right)$$

Staggered control volumes



p is the node
z is the cell

Advancing the nodal velocity components from time *n* to *n*+1 in two steps

$$u^{ps} = u^n + \frac{\Delta t}{M_p} \sum_{i \in p} f_i^n$$

ps = predictor step

$$u^{n+1} = u^n + \frac{\Delta t}{M_p} \sum_{i \in p} \frac{\left(f_i^n + f_i^{ps} \right)}{2}$$

Advancing the internal energy from time *n* to *n*+1 in two steps

$$e^{ps} = e^n - \frac{\Delta t}{M_z} \sum_{i \in z} f_i^n \bullet \frac{\left(u_i^n + u_i^{ps} \right)}{2}$$

$$e^{n+1} = e^n - \frac{\Delta t}{M_z} \sum_{i \in z} \frac{\left(f_i^n + f_i^{ps} \right)}{2} \bullet \frac{\left(u_i^n + u_i^{n+1} \right)}{2}$$

The gradients and nodal forces are calculated using a finite element approach based on the work by Flanagan and Belytschko (1981)

- Position and velocity within a cell are represented in terms of the nodal values and the isoparametric shape functions at the nodes

$$x = \sum_{p \in z} x_p \phi_p(\xi, \eta, \zeta)$$

$$u = \sum_{p \in z} u_p \phi_p(\xi, \eta, \zeta) \qquad \nabla u = \sum_{p \in z} u_p \otimes \nabla \phi_p$$

- The cell center gradient of the velocity is then $\nabla u_z = \frac{1}{V_z} \sum_{p \in z} u_p \otimes \int_{V_z} \nabla \phi_p \, dV = \frac{1}{V_z} \sum_{p \in z} u_p \otimes \hat{B}_p$

$$\frac{\dot{V}_z}{V_z} = tr(\nabla u_z)$$ satisfies GCL

- The force at a node p from the Chaucy stress, $T = \tau - pI$, in cell z is $f_{p(z)} = -T_z \bullet \hat{B}_p$
- The Riemann force at node p from cell z is $f^R_{p(z)} = \varphi_z \mu_{c(p)} \left(u^*_z - u_p \right) \left| \hat{B}_p \bullet a_{c(p)} \right|$
- The anti-hourglass force at a node p from cell z is $f^{HG}_{p(z)}$

A multi-dimensional Riemann-like problem is solved at the cell center to simulate shocks

- The Riemann force for node p is

  Finite element formulation

$$f^R_{p(z)} = \varphi_z \mu_{c(p)} \left(u_z^* - u_p\right) \left|\hat{B}_p \bullet a_{c(p)}\right|$$

  Finite volume formulation

$$f^R_{p(z)} = \varphi_z \sum_{i \in c(p)} \mu_{c(p)} \left(u_z^* - u_p\right) \left|S_i \bullet a_{c(p)}\right|$$

- The shock impedance is $\mu_{c(p)} = \rho_z c_z + b_z \left\| \bar{u}_z - u_p \right\|$
- $a_{c(p)}$ is a unit vector in the direction of $\bar{u}_z - u_p$
- Several limiters considered for reducing dissipation in smooth regions

<u>minmod</u>

$$\varphi_z = \min\left(1, \frac{\nabla \bullet u_\beta}{\nabla \bullet u_z} \right)$$

<u>reduced impedance</u>

$$l = \frac{V^{1/3} \nabla \bullet u_z}{c}$$

$\varphi_z = 0.2$ when l<0.1

The Riemann velocity, u_z^*, is found by summing all Riemann forces from the corner surfaces within the cell

$$\sum_{p \in z} f^R_{p(z)} = 0$$

$$u_z^* = \frac{\sum_{p \in z} \left(u_{c(p)} \mu_{c(p)} \left| \hat{B}_p \bullet a_{c(p)} \right| \right)}{\sum_{p \in z} \left(\mu_{c(p)} \left| \hat{B}_p \bullet a_{c(p)} \right| \right)}$$

Literature examples of multi-dimensional Riemann problems for Lagrangian hydrodynamics (SGH, CCH and PCH)

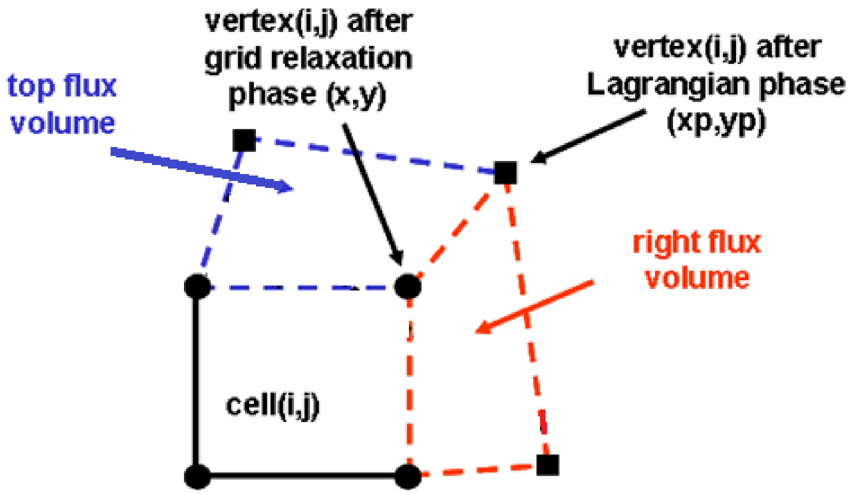
- Despres and Mazeran (Arch. Ration. Mech. Anal. 2005)
- Maire et al. (J. Sci. Compt. 2007)
- Burton et al. (JPC 2013)
- Loubere et al. (Int. J. Numer. Meth. Fluids 2013)
- Morgan et al. (JPC 2015)

ALE is performed by a Lagrange step plus a remap step that conserves total energy

- Flux volumes and associated mass fluxes are illustrated by a 2D mesh

- The remap process is

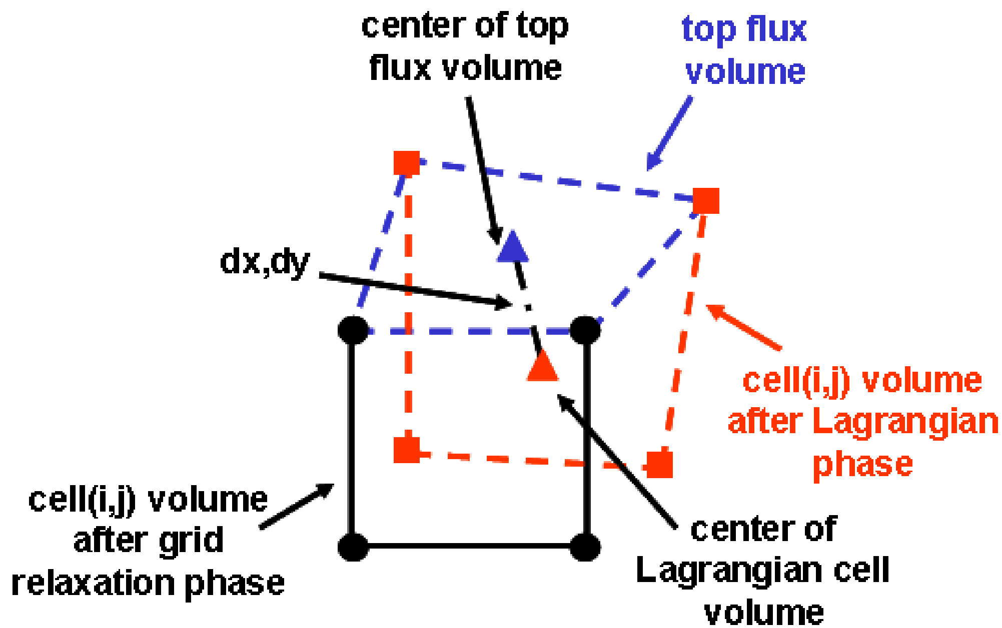
  1. Mesh relaxation moves (xp,yp) to (x,y)
  2. Flux volumes are calculated
  3. Mass fluxes are based on flux volumes and upwind densities
  4. Total energy and internal energy fluxes are calculated using the same flux volumes
  5. Momentum fluxes are calculated on the dual mesh using the mass fluxes from the cell mesh



- The total energy is calculated at the zone center using the nodal kinetic energies and cell center internal energy

The remap fluxes are calculated using a limited second order reconstruction

- 2D example of a higher order mass flux calculation for the top flux volume



$$M^A = \underbrace{\rho_{upwind}}_{\text{donor cell method}} V^A + V^A \left[dx \frac{\partial \rho}{\partial x}_{upwind} \underbrace{+}_{\text{correction}} dy \frac{\partial \rho}{\partial y}_{upwind} \right]$$

Superscript A denotes advected

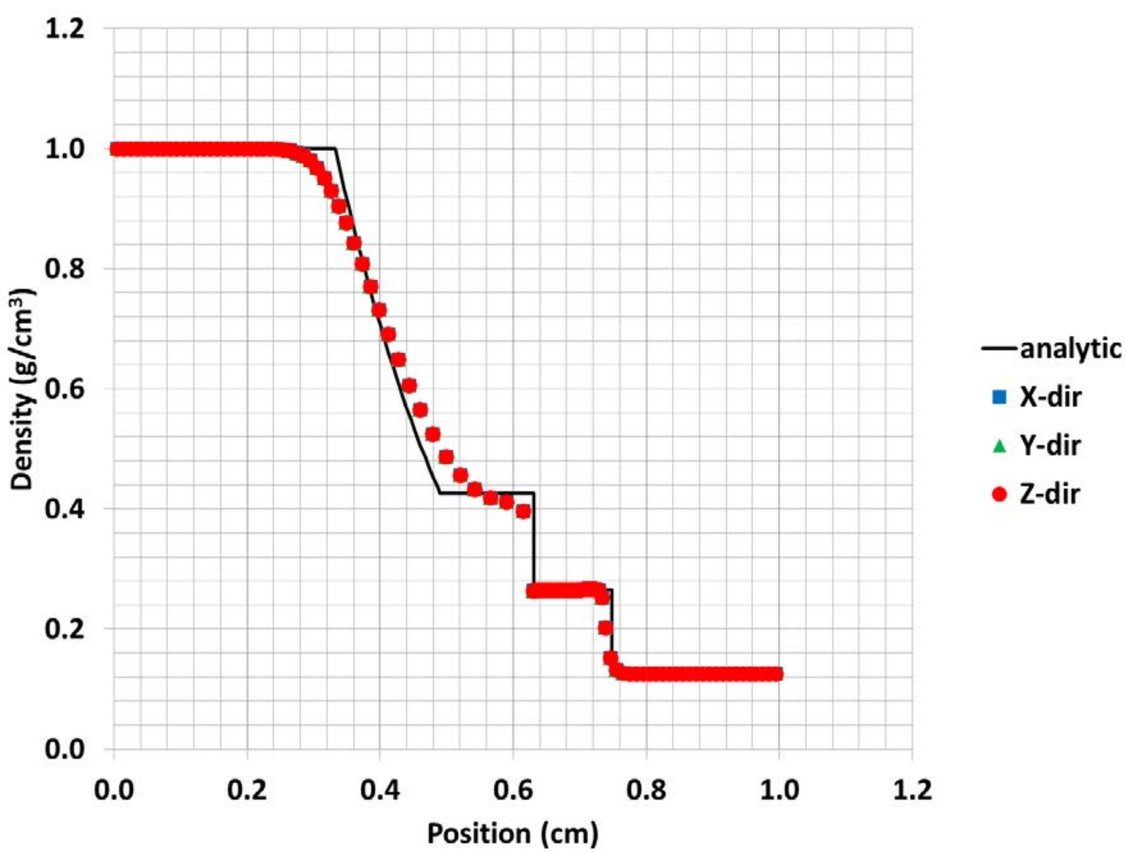
Barth Jespersen method for calculating the density gradient

Lagrangian Test Problems

The locations of the shock and contact discontinuity for the Sod test problem are captured by the code

Setup

- An initial discontinuity between two ideal gas regions (γ=1.4)
- Region 1
  - density of 1 g/cm^3
  - pressure of 1 Mbar
- Region 2
  - density of 0.125 g/cm^3
  - pressure of 0.1 Mbar
- 100 cells
- The solution is obtained at 0.1415 μs



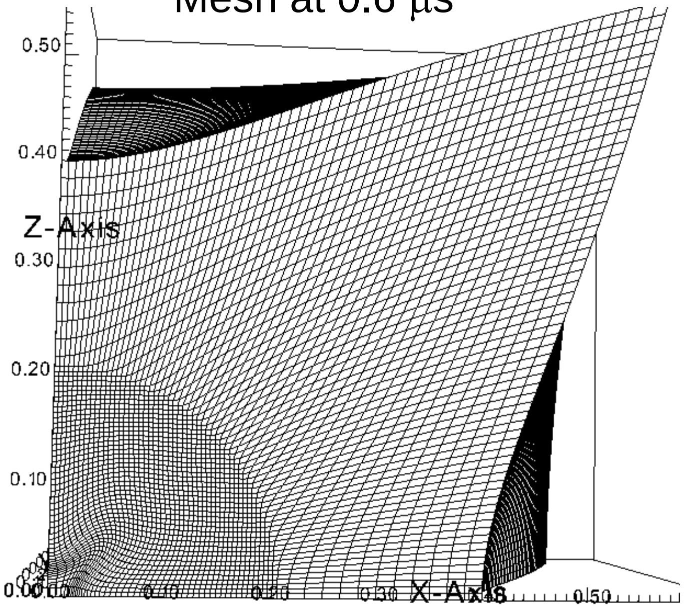
The expansion fan is a bit diffusive owing to the Riemann problem being active in expansion

The 3D Noh problem demonstrates the accuracy and symmetry preservation of the new approach

Setup

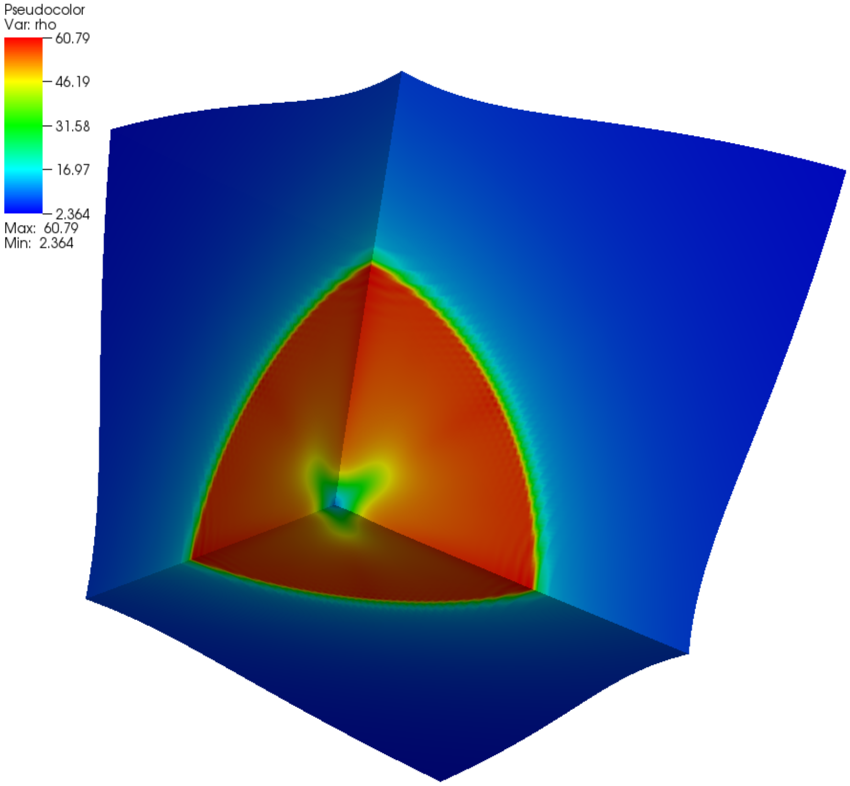
- 1 cm octant with 60 x 60 x 60 cells
- 1 cm/μs initial velocity directed toward the origin
- Uniform initial pressure of zero and density of 1 g/cm^3
- Ideal gas with γ=5/3

Mesh at 0.6 μs



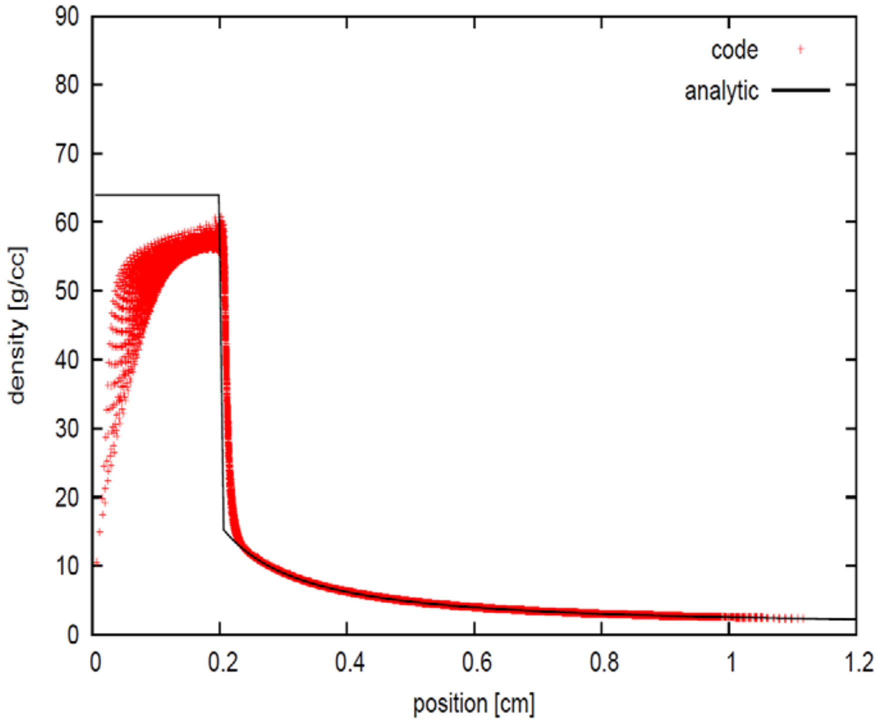
Density contours at 0.6 μs

Density (g/cm^3)

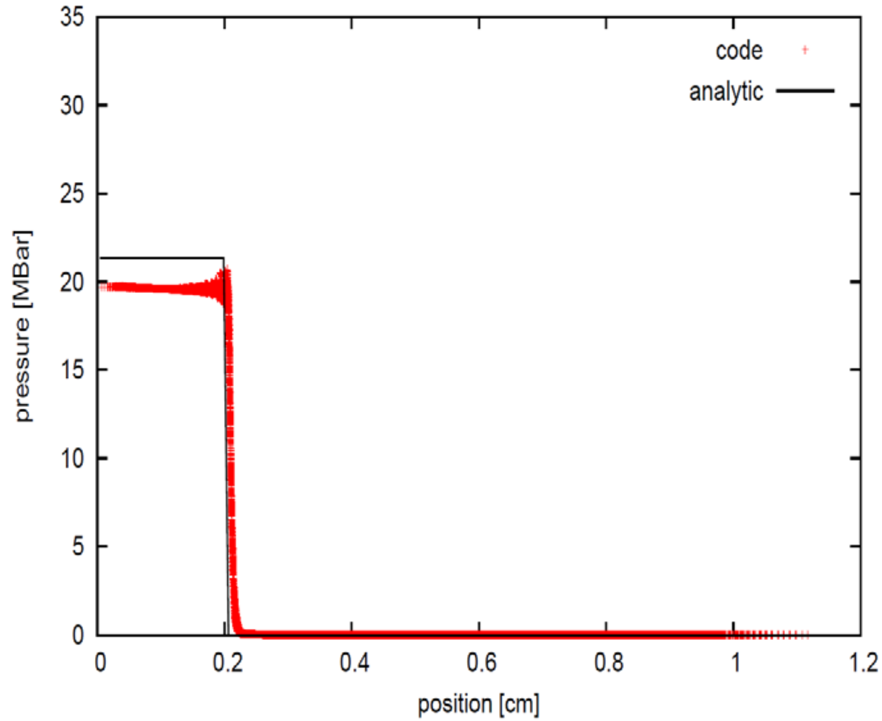


Numerical results for the 3D Noh problem show little scatter

Density



Pressure

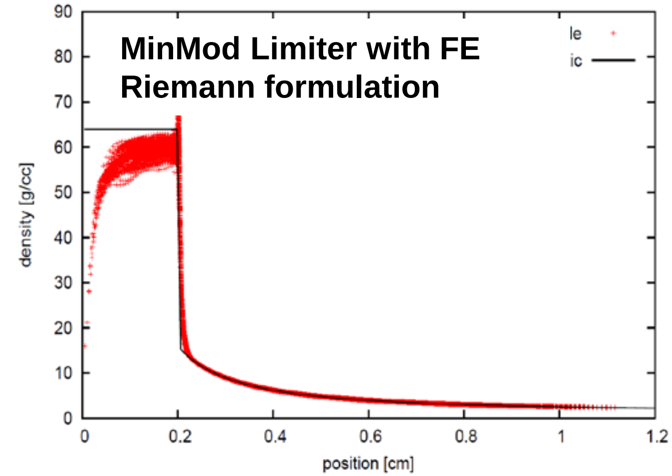


Red denotes the calculated solution at 0.6 μs including all cell-centered values on the mesh

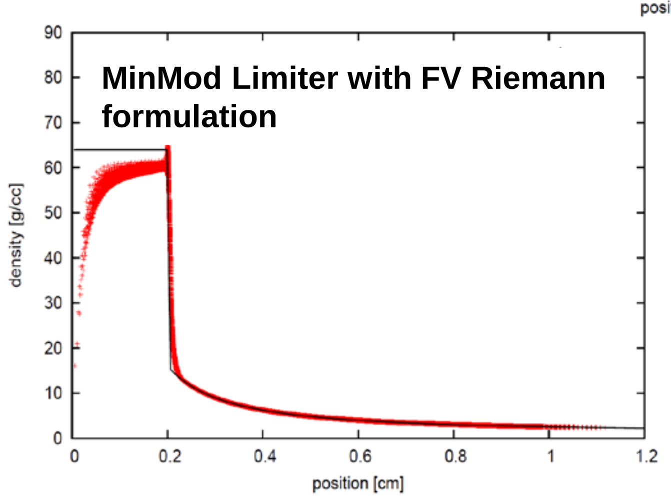
Reduced limiter and finite volume (FV) Riemann formulation

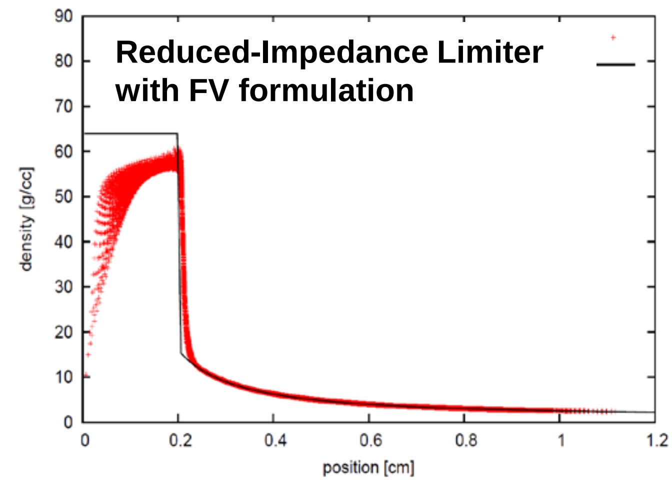
The finite volume Riemann formulation gives better density results for the 3D Noh problem

Red denotes the calculated solution at 0.6 μs including all cell-centered values on the mesh



FV = finite volume
FE = finite element

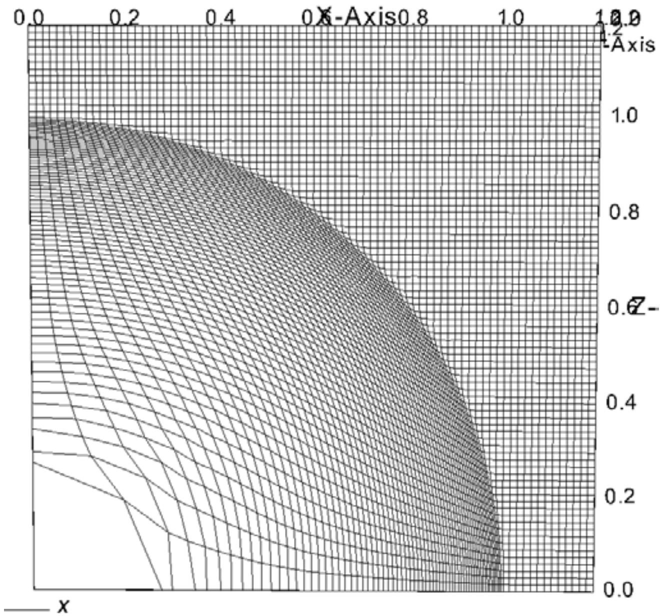




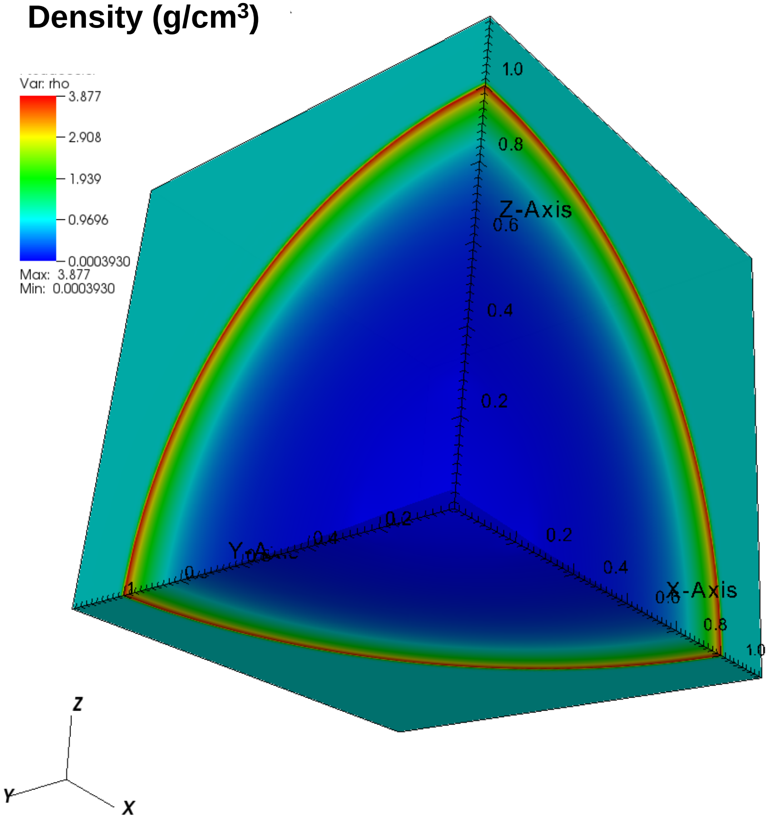
The results for the 3D Sedov blast wave problem demonstrate the accuracy and mesh robustness of the new approach

- An ideal gas (γ=5/3)
- A 1.2 cm octant (80 x 80 x 80 cells)
- Energy source at the origin
  - 56 kJ
- The solution is obtained at 1.0 μs

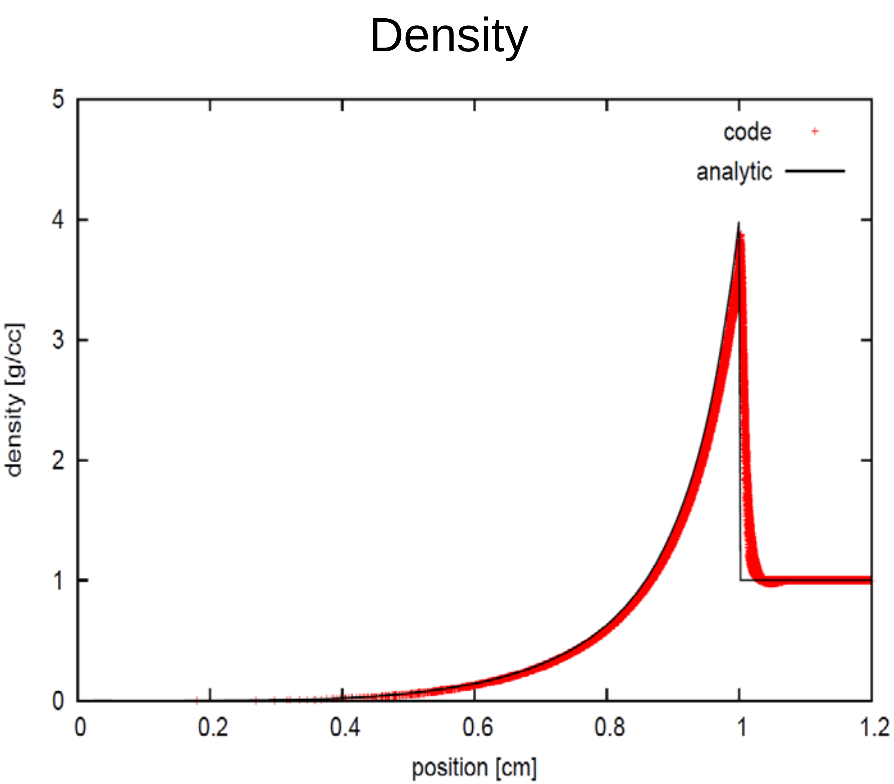
Mesh at 1.0 μs

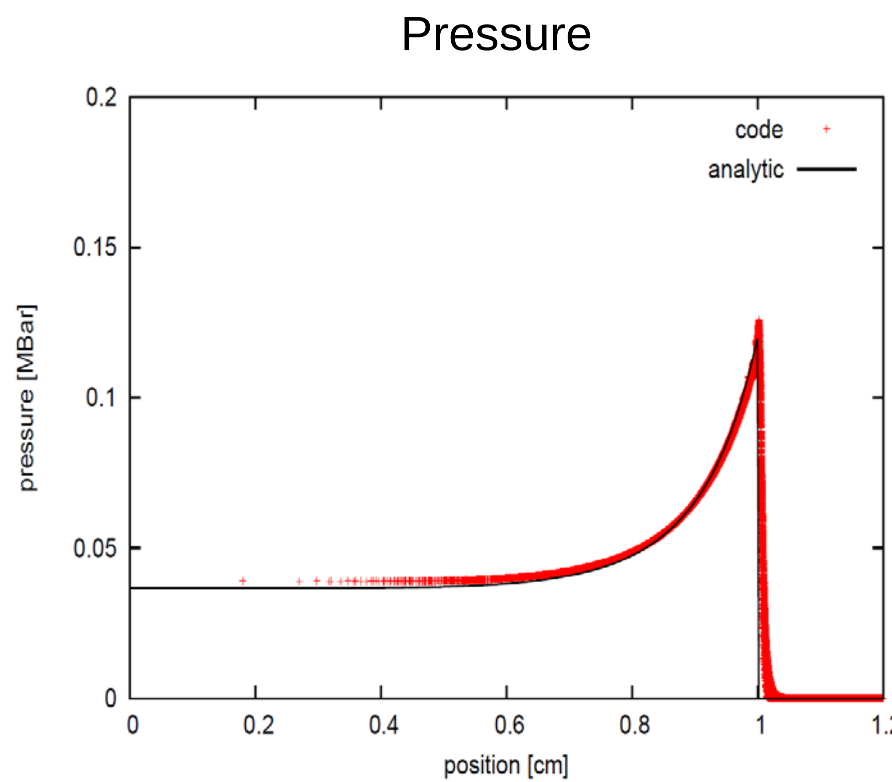


Density contours for 3D Sedov problem at 1.0 μs



The calculated blast front follows the analytic solution and the symmetry of the front is good

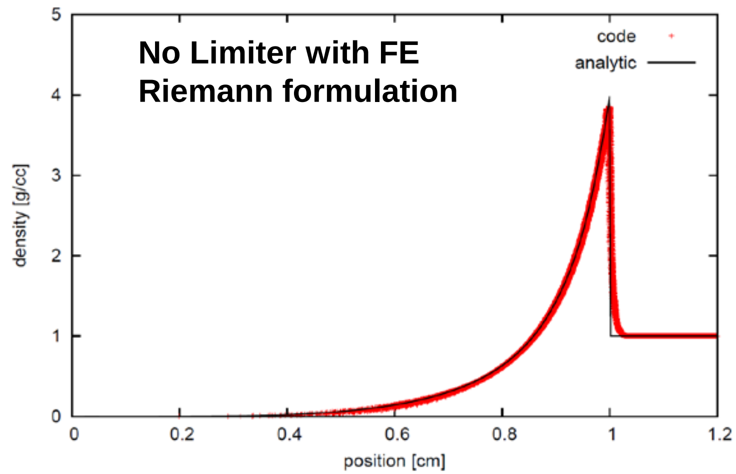


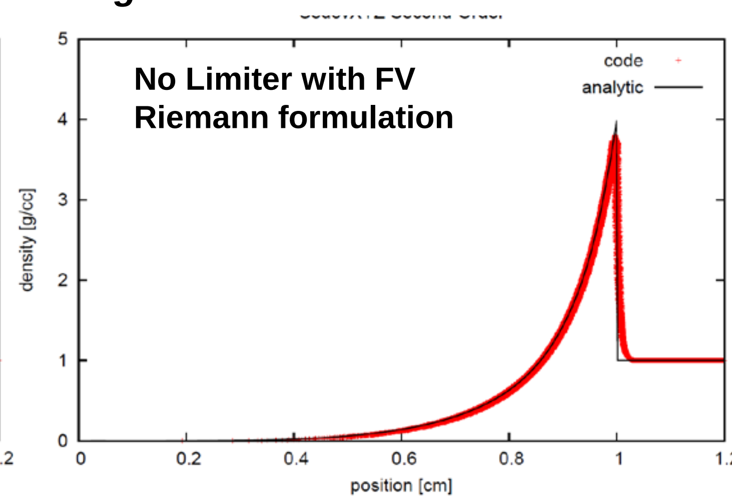


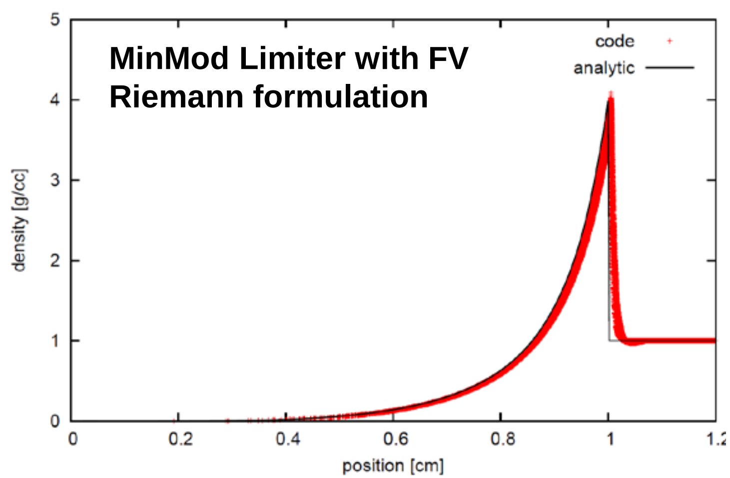
Red denotes the calculated solution at 1 μs including all cell-centered values on the mesh

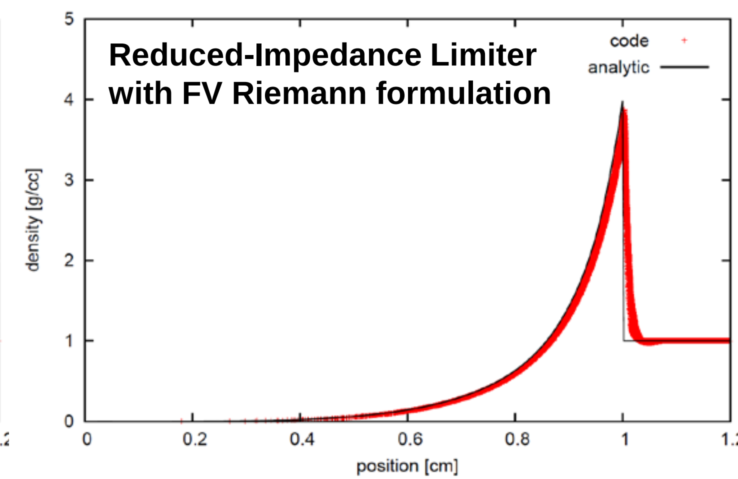
Different limiters and Riemann formulations give virtually the same density for the 3D Sedov problem

Red denotes the calculated solution at 1 μs including all cell-centered values on the mesh









The results for the Verney problem show our approach can accurately convert kinetic energy into internal energy for a constant density implosion

- Imploding steel shell
  - inner radius of 8 cm
  - 0.5 cm thick
- Initial velocity profile

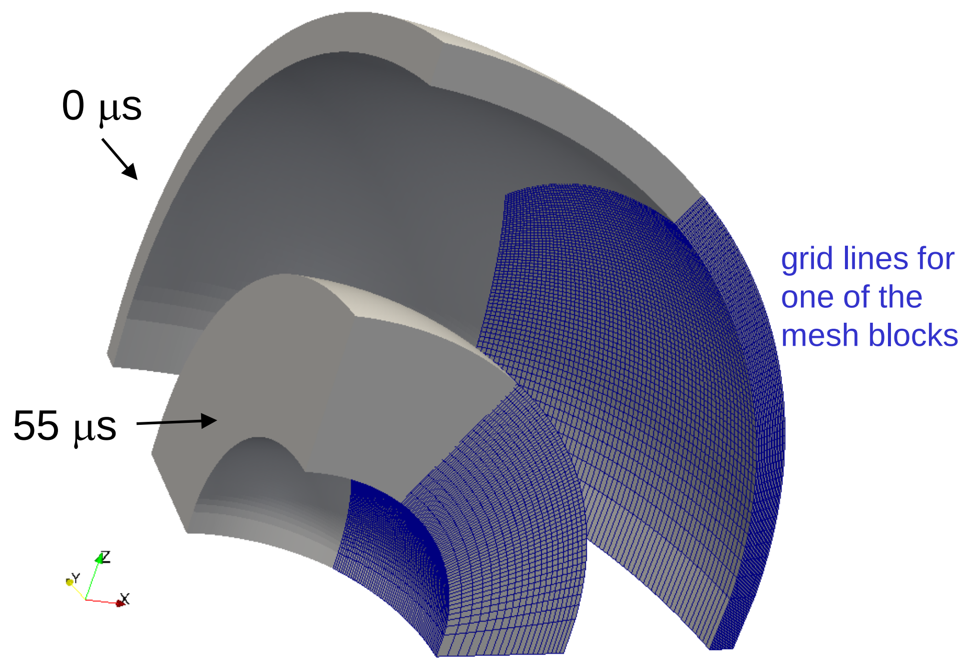
$$u = u_0^2 (r_0 / r)^2$$

  - u_0=0.14 cm/μs
  - results in constant density implosion
- Simple strength model
  - shear modulus, μ=0.895 Mbar
  - yield stress of 0.050 Mbar
- Gruneisen EOS

ρ_0=7.90
C_0=0.457
S_1=1.49
γ_0=1.93
b=0.50

- Analytic solution from Weseloh (2007)

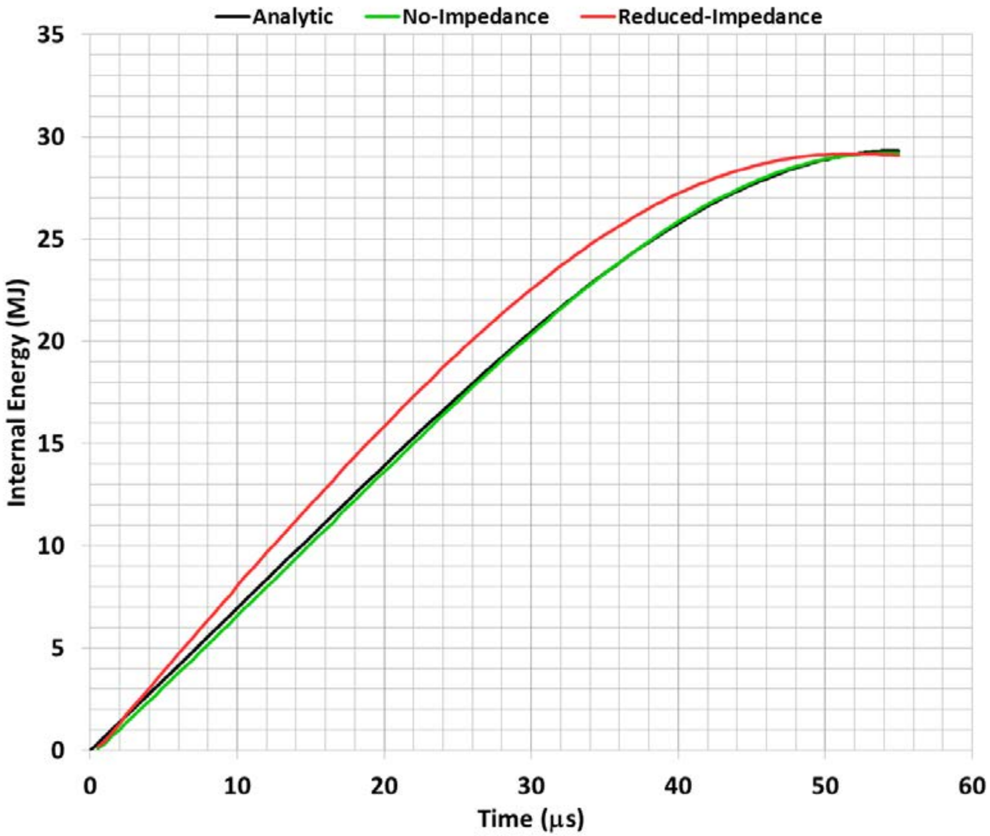
Computational mesh for the Verney test problem at 0 μs and 55 μs



- 3 mesh blocks with 64 x 64 x 20 cells each
- Parallelization using OpenMP

The calculated internal energy history of the shell agrees very well with the analytic solution for the case when the Riemann solution is omitted

Internal Energy of the Shell

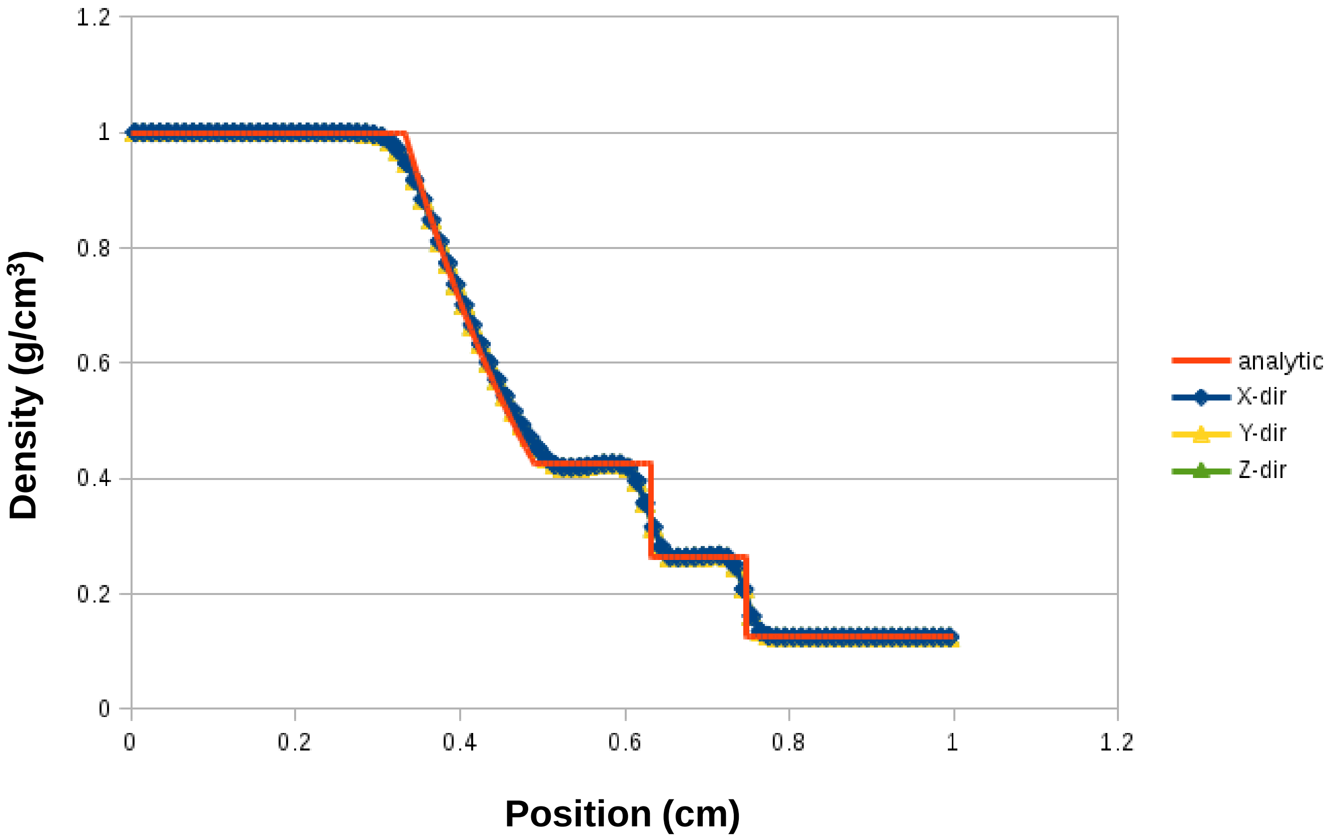


3 mesh blocks with 16 x 16 x 20 cells each

- The calculation without the Riemann solution (no-impedance case) closely follows the analytic solution
- The reduced impedance limiter achieves the correct final internal energy but has excess internal energy during the implosion

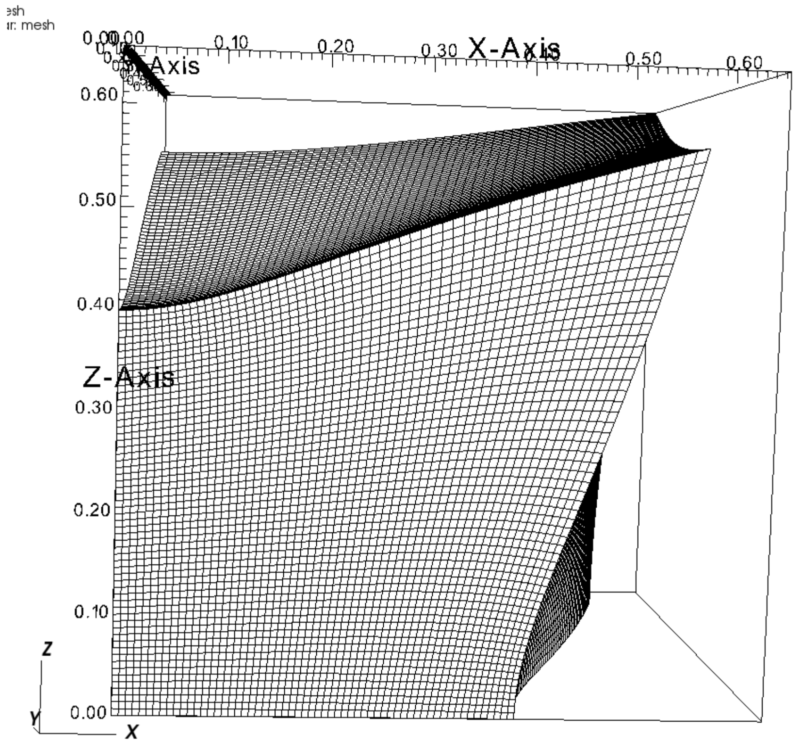
ALE Test Problems

The calculated densities for the Sod problem are improved by using ALE

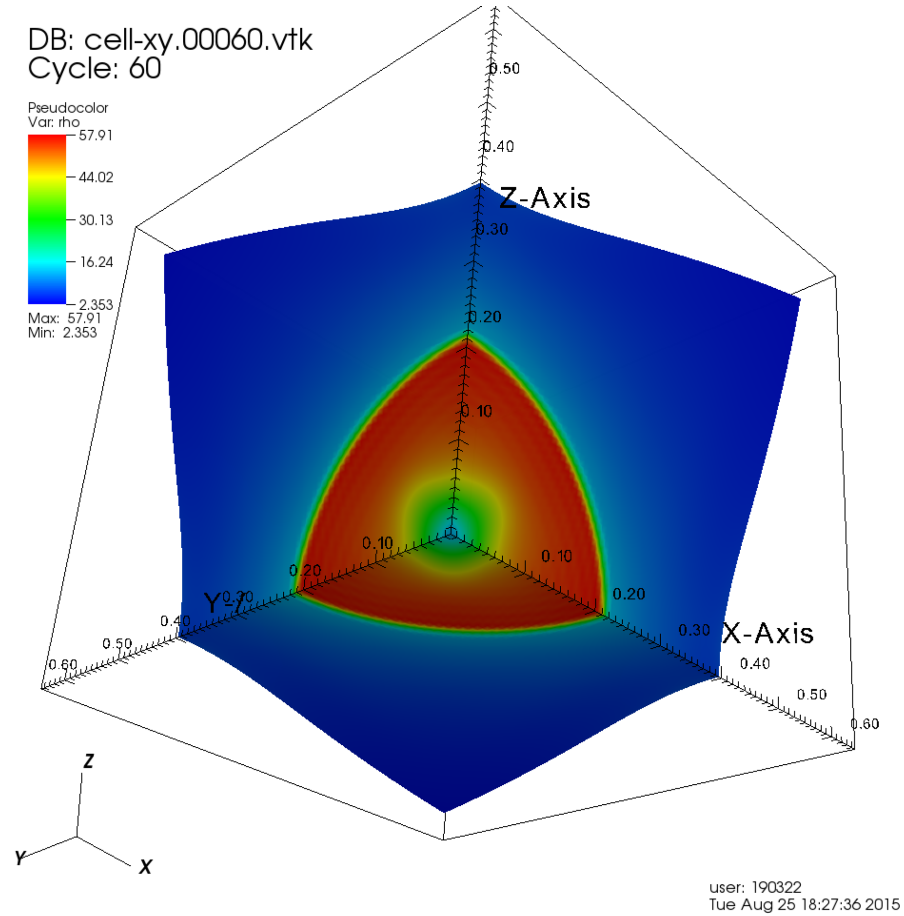


Excellent results were achieved for the 3D Noh problem using ALE

Mesh at 0.6 μs



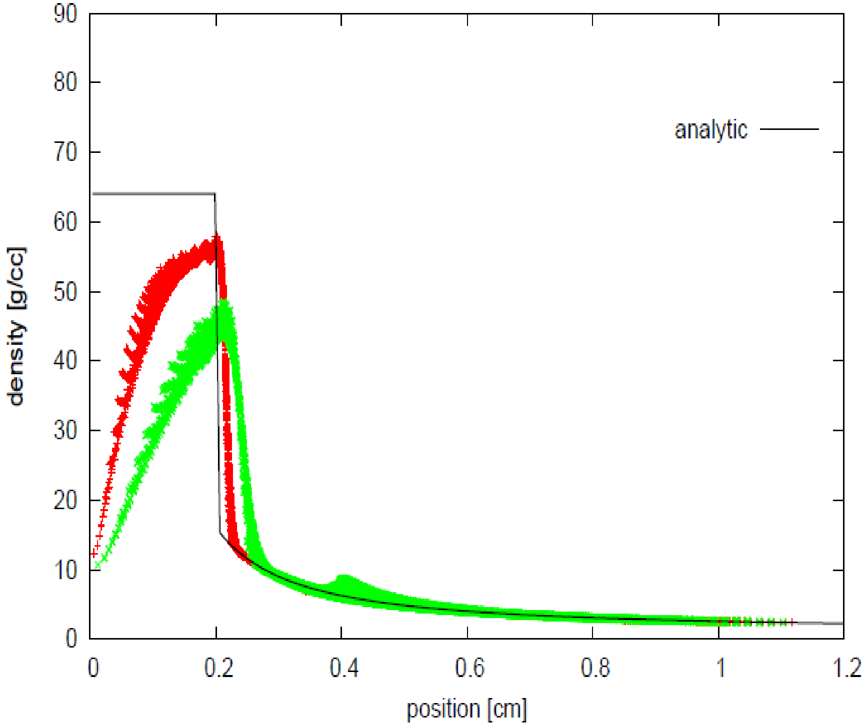
Density contours at 0.6 μs



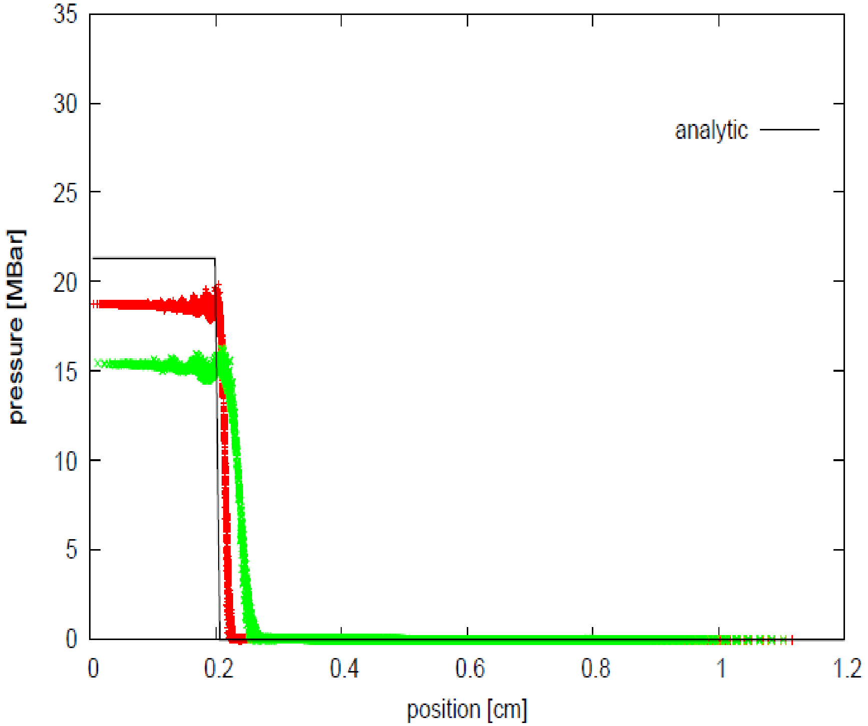
The mesh was continuously relaxed using the 3D Winslow algorithm

3D Noh problem results using ALE had excellent symmetry with very little scatter

Density



Pressure

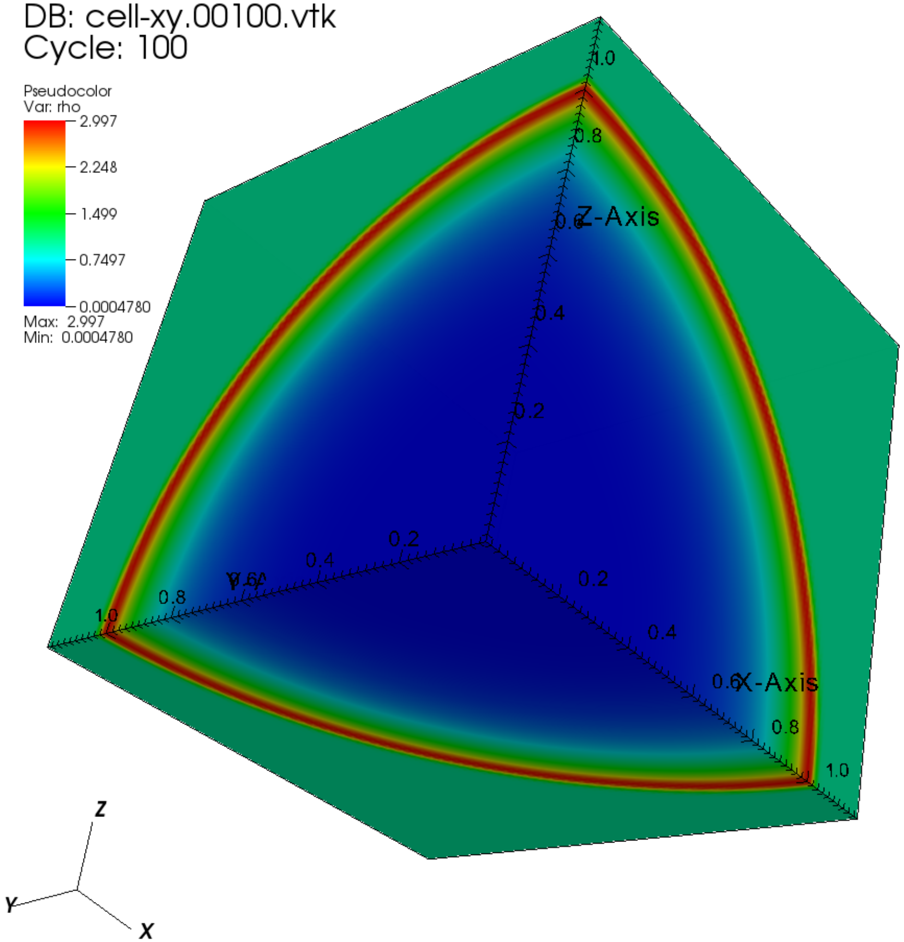


The calculated solution is shown at 0.6 μs including all cell-centered values on the mesh

Red denotes a 60 by 60 by 60 mesh
Green denotes a 30 by 30 by 30 mesh

The 3D Sedov blast wave calculation using ALE shows excellent symmetry and great mesh robustness

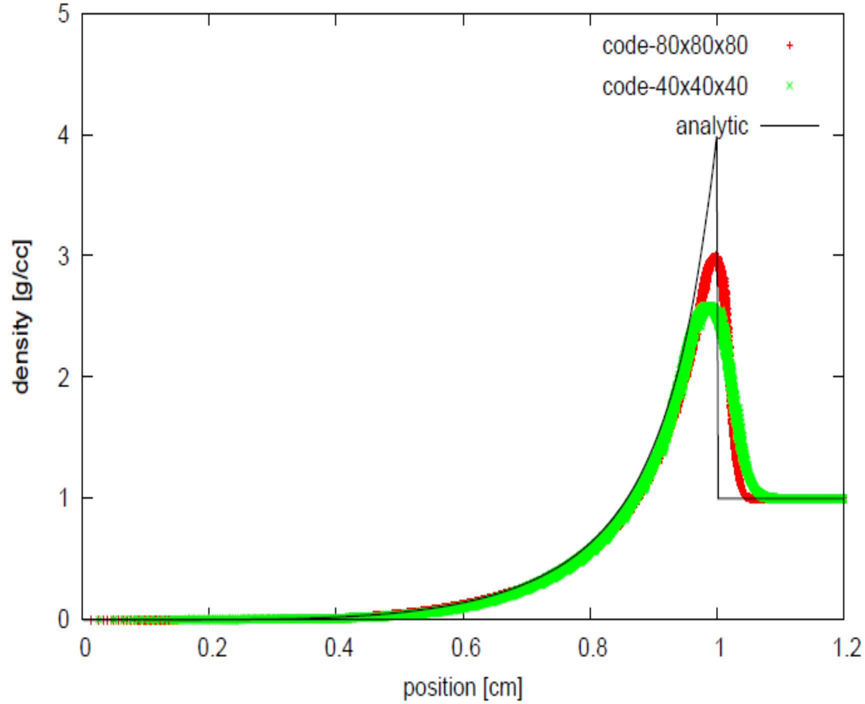
Density contours for 3D Sedov problem at 1.0 μs



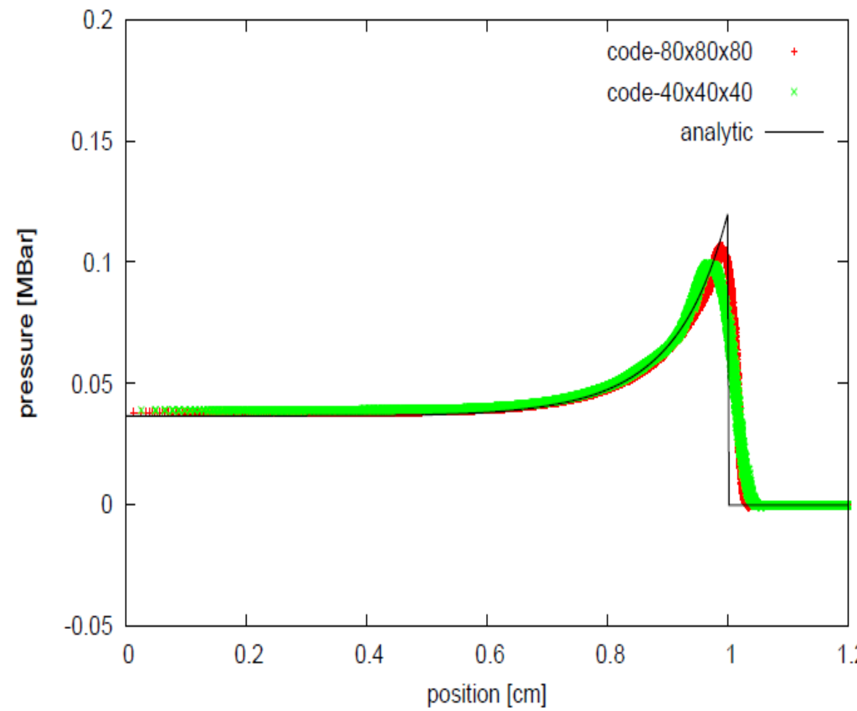
A constant Eulerian mesh was used for the simulation

The 3D Sedov problem results using ALE had excellent symmetry with very little scatter

Density



Pressure



The calculated solution is shown at 1 μs including all cell-centered values on the mesh

Red denotes a 80 by 80 by 80 mesh
Green denotes a 40 by 40 by 40 mesh

The Taylor Green vortex results demonstrate that the Lagrangian method is robust to extreme mesh distortion

- Unit density
- An ideal gas (γ=5/3)
- A 2D mesh (40 by 40 by 1 cells)
- Riemann solution is omitted

Initial conditions

$$u^{t=0} = \sin(\pi x)\cos(\pi y)$$

$$v^{t=0} = -\cos(\pi x)\sin(\pi y)$$

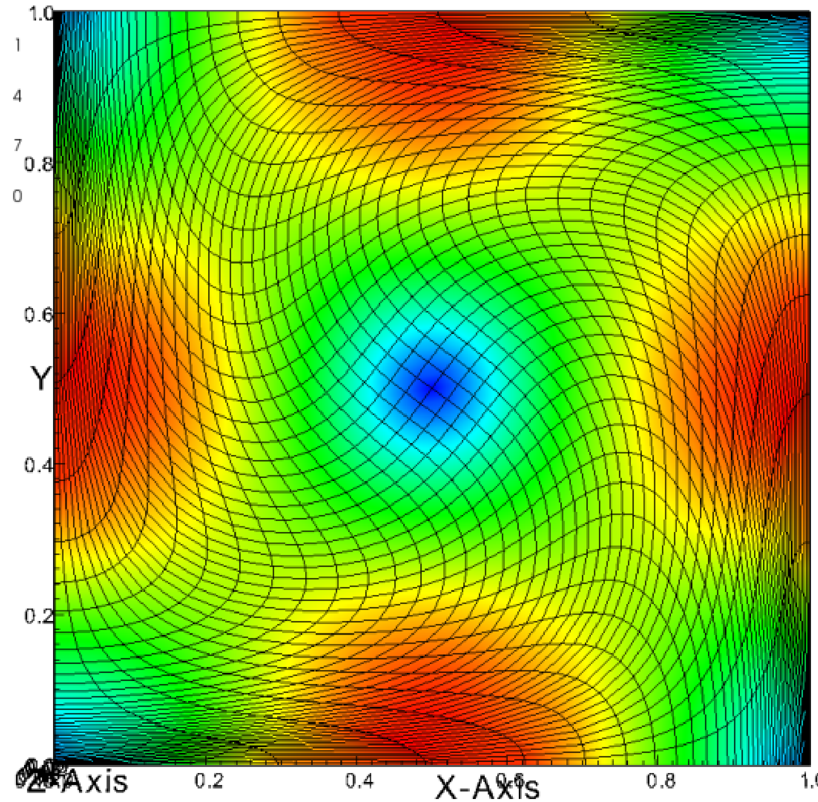
$$w^{t=0} = 0$$

$$p^{t=0} = 10 + \frac{1}{4}\left(\cos(2\pi x) + \cos(2\pi y)\right)$$

Energy source term

$$S_E = \frac{3\pi}{8}\left[\cos(\pi x)\cos(3\pi y) - \cos(3\pi x)\cos(\pi y)\right]$$

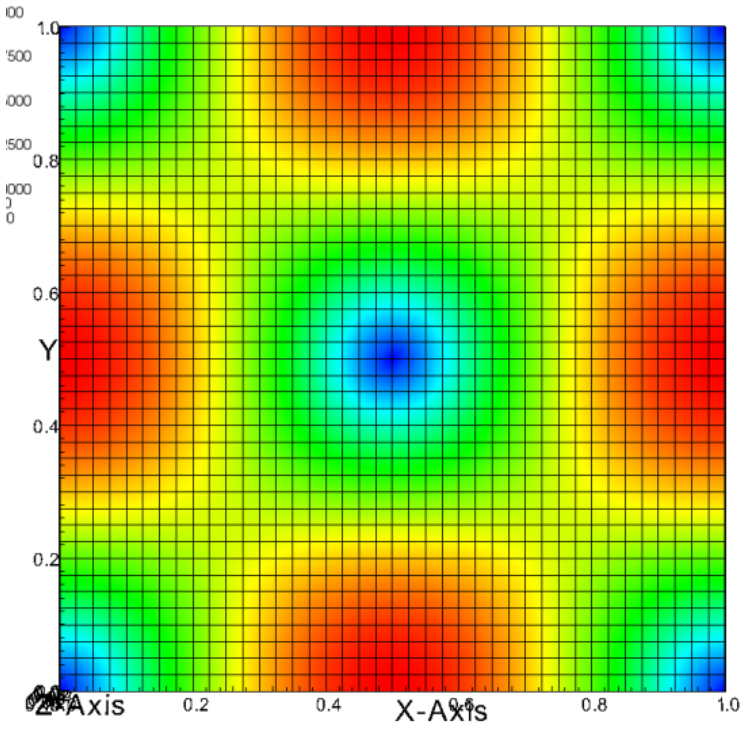
Lagrangian solution for velocity magnitude at 0.8 μs



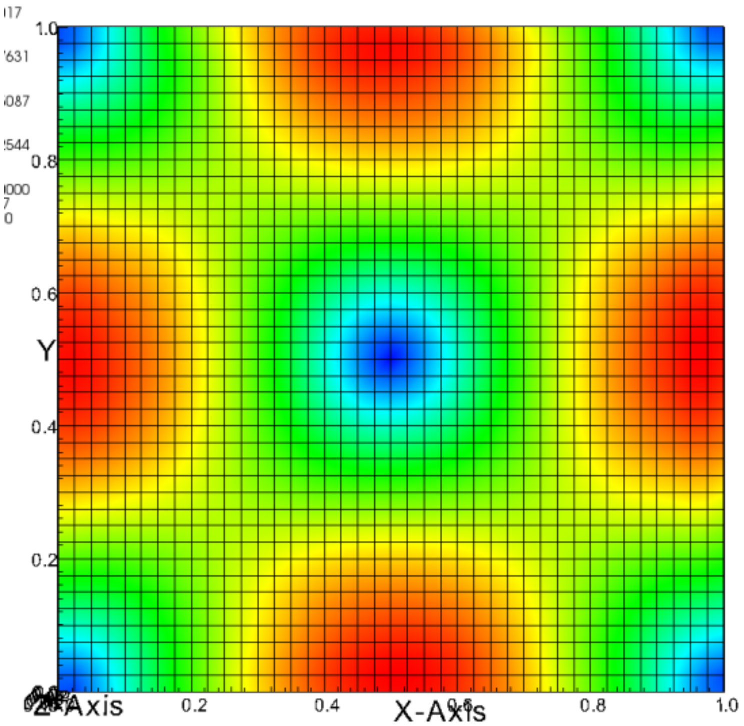
Our underlying Lagrangian method is robust to extreme mesh distortion

Our ALE method does a good job of preserving the initial velocity field

Velocity magnitude at 0 μs

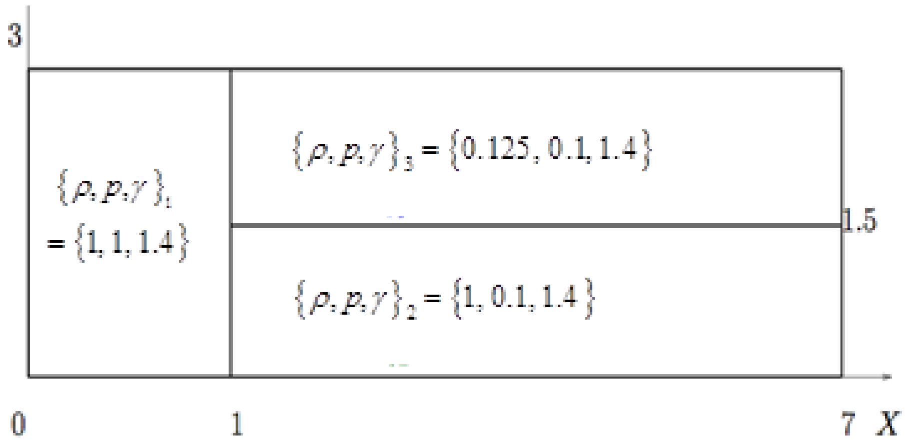


Velocity magnitude at 0.8 μs



The triple point problem has significant vorticity, large shear and complex interacting shocks

Initial geometry and conditions



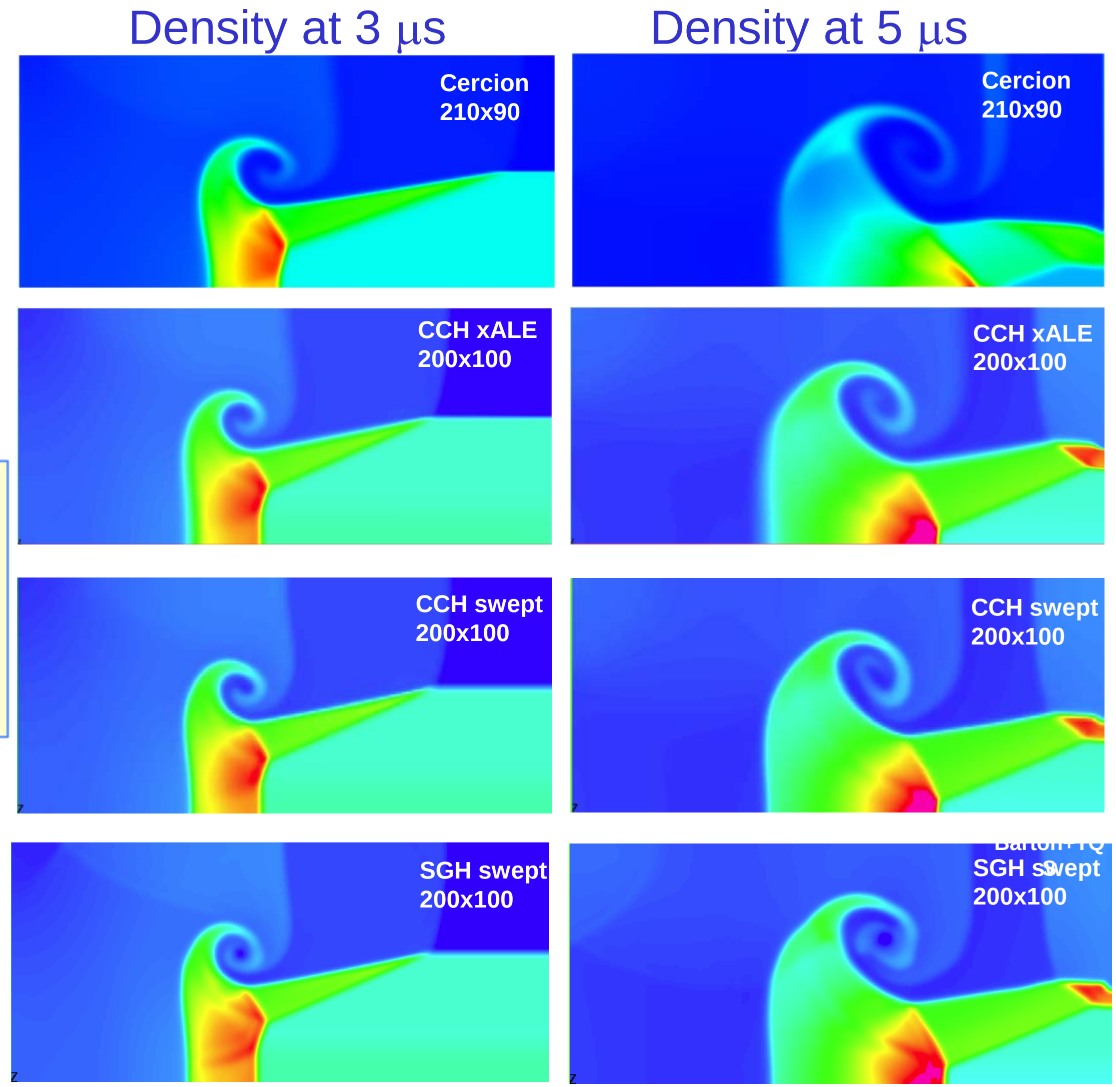
- *Gamma law gas*
- *A single material with three regions*
- *A high pressure region drives a shock through two connected regions*
- *A vortex develops at the triple point*
- *2D mesh*

Cercion 3D with ALE produces less vorticity and different hydrodynamics at late time compared with other CCH and SGH methods

- Cercion 3D leads the other methods by about 0.5 μs
- CCH and SGH results taken from Burton et al. LA-UR-13-24119

CCH is a new cell-centered alternative to Lagrangian Staggered Grid Hydro (SGH)

xALE is ALE based upon an exact intersection remap – an alternative to traditional swept face methods



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Conclusions

- A multi-dimensional Riemann solution has been applied together with a classical finite element approach for Lagrangian hydrodynamics in our Cercion 3D code
- A total energy conserving remap using Barth Jesperson gradients
- Lagrangian results with reduced impedance limiter
  - The expansion fan in the Sod problem is a bit diffusive with the Riemann problem active in expansion
  - The calculated Sedov blast front follows the analytic solution and the symmetry of the front is good
  - The correct final internal energy for the Verney imploding shell is achieved but there are errors in the internal energy during the implosion
- ALE results
  - Better calculated densities for the Sod problem than with the Lagrangian method
  - Excellent symmetry for the 3D Sedov blast wave
  - A good job of preserving the initial velocity field in the Taylor Green vortex problem
  - We have less vorticity and different hydrodynamics at late time for the triple point problem compared with other CCH and SGH methods