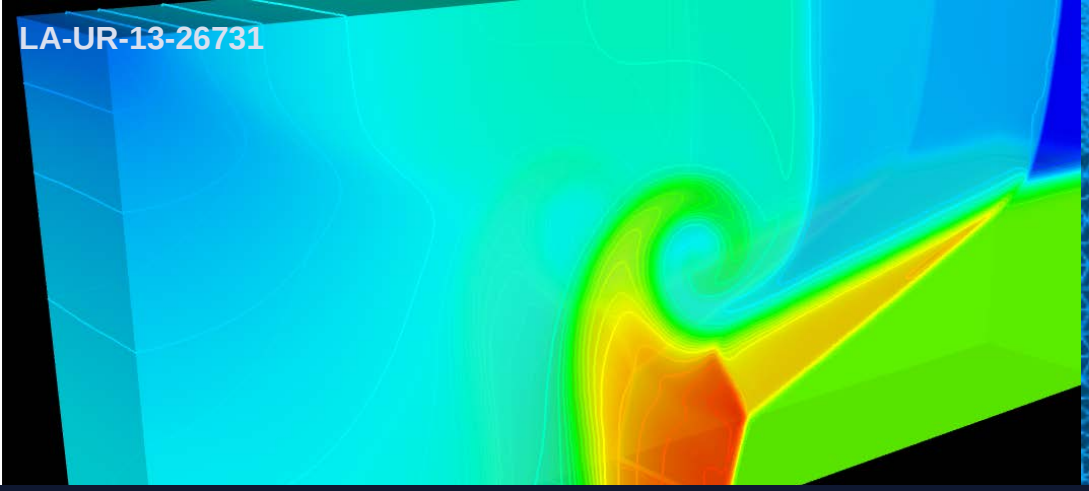
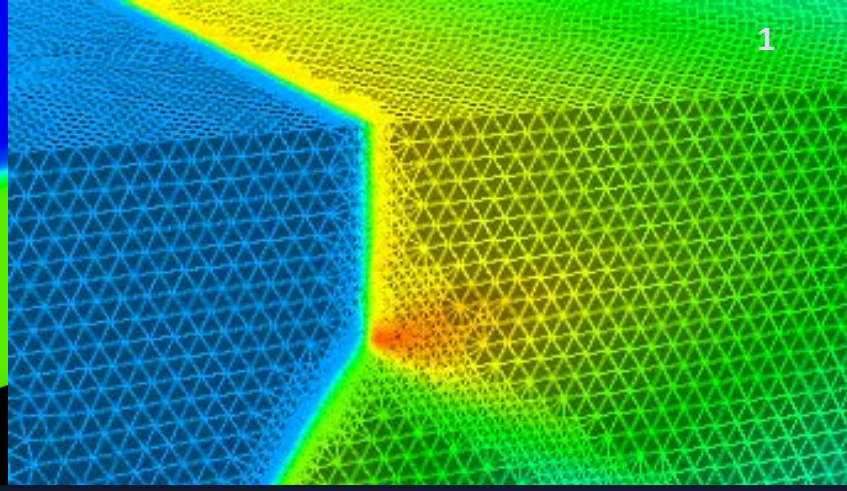
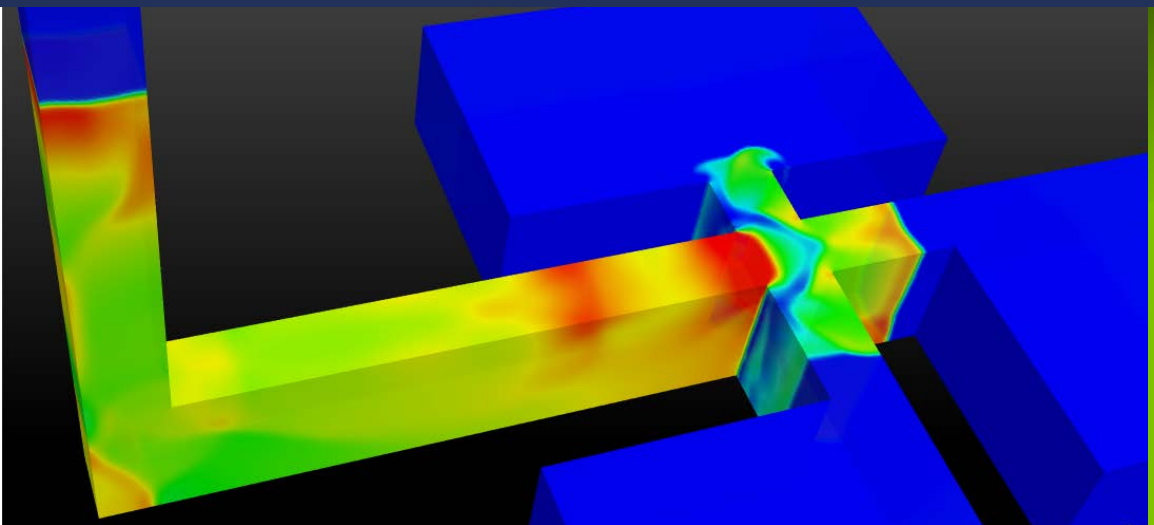


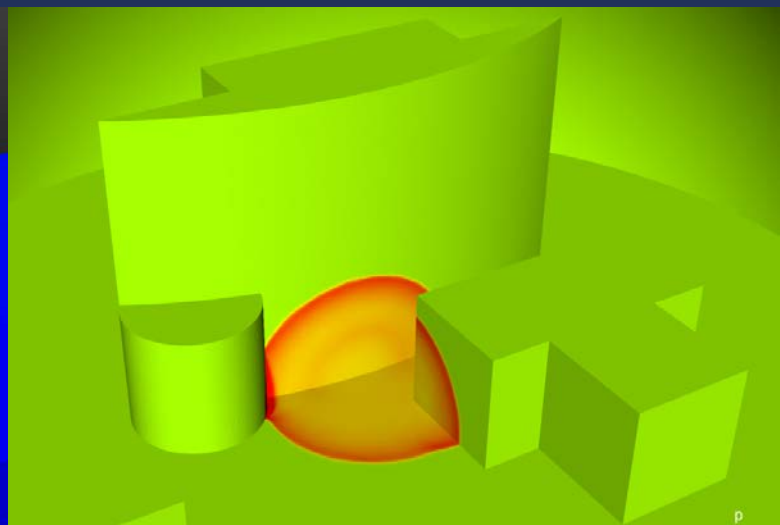


OPERATOR SPLITTING AND TIME ACCURACY IN LAGRANGE PLUS REMAP METHODS

The CHICOMA Project

J. Waltz (PI), T. Canfield, M. Charest, N. Morgan, D. Risinger, and J. Wohlbier





The time accuracy characteristics of the Lagrange-plus-remap ALE method have been investigated

- The standard Lagrange-plus-remap method is shown, both analytically and numerically, to be 1st-order accurate in time
  - Errors result from operator splitting and low-order time integration of remap terms
  - Errors exist even if the underlying Lagrange step is 2nd-order accurate in time
- A 2nd-order accurate (in time) ALE method can be achieved with an unsplit treatment of the remap terms
  - Improvements to the Lagrange-plus-remap method also are possible
- Application of unsplit ALE to 3D shock hydrodynamics is demonstrated on unstructured meshes of up to 10^7 tetrahedra
  - The method satisfies the Geometric Conservation Law to truncation error
  - Convergence under mesh refinement is observed at the expected order of accuracy

We are investigating unsplit flux-conservative ALE methods due to several benefits over Lagrange-plus-remap methods

- Temporal errors due to operator splitting are eliminated
  - Single high-order time integrator for all terms in the right-hand-side
- Computational cost is reduced
  - One pass over the mesh versus two
- Consistent spatial discretization for all terms in the right-hand-side
  - Everything converges at the same rate
- The discrete system is exactly conservative by construction
  - Lax-Wendroff theorem: If the solution converges, then it will converge to a proper weak solution of the conservation law
- Approximate Riemann solvers are readily incorporated
  - Eliminates need for artificial viscosity treatments

This talk focuses on time accuracy issues associated with operator splitting and the application of unsplit ALE methods to 3D shock hydrodynamics.

Operator splitting errors and concepts can be illustrated with a simple ODE

- Linear, first-order ODE: $\frac{dy}{dt} = Ay + By$

  Exact solution: $y(t) = e^{(A+B)t}$

- Lie splitting ("A then B"): solve $\frac{dy}{dt} = Ay$ followed by $\frac{dy}{dt} = By$

  Exact solution: $y(t) = e^{At}e^{Bt}$

  Splitting error: $\epsilon = e^{(A+B)t} - e^{At}e^{Bt} = \frac{t^2}{2}[B,A] + \frac{t^3}{12}\left([B,[B,A]] - [A,[A,B]]\right) + O(t^4)$

- General nonlinear case: $\frac{dy}{dt} = f(y) + g(y) + \cdots$ follows from Baker-Campbell-Hausdorff formula

Lie splitting is 1st-order accurate even if A and B can be integrated exactly!
(Unless A and B commute, but that is not a very interesting problem)

Strang's method has been widely used to achieve a 2nd-order accurate operator split

- Strang splitting:
  - Solve $\frac{dy}{dt} = Ay$ over *[0,t/2]*
  - Solve $\frac{dy}{dt} = By$ over *[0,t]*
  - Solve $\frac{dy}{dt} = Ay$ over *[t/2,t]*

Exact solution: $y(t) = e^{At/2}e^{Bt}e^{At/2}$

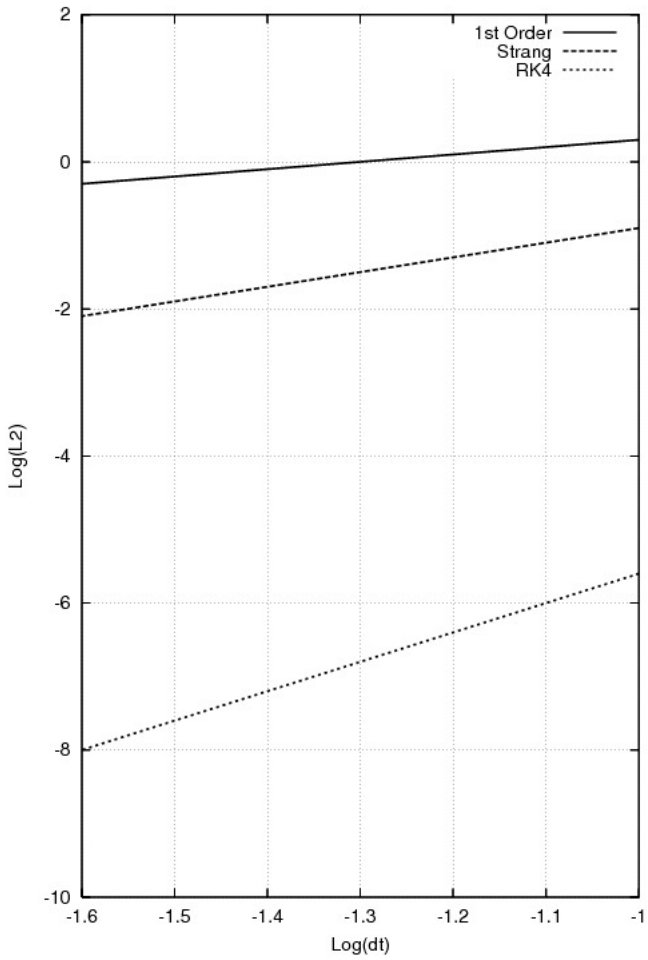
Splitting error: $\epsilon = e^{(A+B)t} - e^{At/2}e^{Bt}e^{At/2} = t^3\left(\frac{1}{12}[B,[B,A]] - \frac{1}{24}[A,[A,B]]\right) + O(t^4)$

Strang splitting is *2nd-order accurate* but requires more computational work since *A* (or *B*) must be evaluated twice per time step.

These errors are trivially demonstrated numerically

- Example ODE: $\frac{dy}{dt} = -y^3 - 2ty^2$

- Integrate with three methods:
  - Lie splitting + RK4 on each operator
  - Strang splitting + RK4 on each operator
  - Unsplit RK4
- Measure self-convergence relative to unsplit, small-Δt result
- Average convergence rates are exactly as expected:
  - Lie: 1.05
  - Strang: 2.0
  - Unsplit: 4.1



The potential for operator splitting in hydrodynamics can be seen in the ALE form of the equations

- "Eulerian-ALE" equations: transform Eulerian equations to mesh frame

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho u_i\\ \rho E\end{pmatrix}+\frac{\partial}{\partial x_j}\begin{bmatrix}\rho u_j\\ \rho u_i u_j+p\\ \rho E u_j+p u_j\end{bmatrix}=0$$

$$\left[\frac{\partial}{\partial t}\right]_w=\frac{\partial}{\partial t}+w_j\frac{\partial}{\partial x_j}$$

Relation between lab frame and co-moving mesh frame

$$\frac{1}{V}\frac{\partial}{\partial t}\left[V\begin{pmatrix}\rho\\ \rho u_i\\ \rho E\end{pmatrix}\right]_w+\frac{\partial}{\partial x_j}\begin{bmatrix}\rho(u_j-w_j)\\ \rho u_i(u_j-w_j)+p\\ \rho E(u_j-w_j)+p u_j\end{bmatrix}=0$$

- "Lagrangian-ALE" equations: transform Lagrangian equations to mesh frame

$$\frac{Dm}{Dt}=0,\qquad \rho\frac{Du_i}{Dt}=-\frac{\partial p}{\partial x_i},\qquad \rho\frac{De}{Dt}=-p\frac{\partial u_i}{\partial x_i}$$

$$\left[\frac{\partial}{\partial t}\right]_w=\frac{D}{Dt}-(u_j-w_j)\frac{\partial}{\partial x_j}$$

Relation between fluid frame and co-moving mesh frame

$$\left[\frac{\partial m}{\partial t}\right]_w-(u_j-w_j)\frac{\partial m}{\partial x_j}=0$$

$$\rho\left[\frac{\partial u_i}{\partial t}\right]_w+\frac{\partial p}{\partial x_i}-\rho(u_j-w_j)\frac{\partial u_i}{\partial x_j}=0$$

$$\rho\left[\frac{\partial e}{\partial t}\right]_w+p\frac{\partial u_i}{\partial x_i}-\rho(u_j-w_j)\frac{\partial e}{\partial x_j}=0$$

We will show that the Lagrange-plus-remap method is an operator split solution of the Lagrange-ALE equations.

The solution at a zone (or control volume) is modified by both Lagrange and remap steps over the course of a time step

- Typical Lagrange step: n to *
  1. Coordinate half-step

$$x_i^{n+1/2} = x_i^n + \frac{1}{2}\Delta t u_i^n$$

  2. Pressure and forces

$$p^{n+1/2} = f\left(p^n, x_i^{n+1/2}\right)$$

$$F_i^{n+1/2} = -\int_A p^{n+1/2} dA_i$$

  3. Velocity, energy, and coordinate update

$$u_i^* = u_i^n + \frac{\Delta t}{m^n} F_i^{n+1/2}$$

$$e^* = e^n + \frac{\Delta t}{2m^n} F_i^{n+1/2}(u_i^* + u_i^n)$$

$$x_i^* = x_i^n + \frac{1}{2}\Delta t(u_i^* + u_i^n)$$

- Typical remap step: * to n+1
  1. Calculate relaxation displacements and flux volumes

$$\delta x_i^* = f(x_i^*)$$

$$\delta V^* = f(\delta x_i^*)$$

  2. Mass, momentum, energy, and coordinate updates

$$m^{n+1} = m^* + \sum_f \rho^* \delta V^*$$

$$u_i^{n+1} = u_i^* + \frac{1}{m^{n+1}} \sum_f (\rho u_i)^* \delta V^*$$

$$e^{n+1} = e^* + \frac{1}{m^{n+1}} \sum_f (\rho e)^* \delta V^*$$

$$x_i^{n+1} = x_i^* + \delta x_i^*$$

Although details and notation may vary, those variations don't change the fact that both procedures modify the solution at each time step.

The terms can be combined to give the full expression for a single time step

- Mass, momentum, energy, and coordinate updates (after a bit of manipulation and dividing both sides by Δt):

$$\frac{m^{n+1}-m^n}{\Delta t}-\frac{1}{\Delta t}\sum_f \rho^*\,\delta V^*=0 \qquad \left\lfloor\frac{\partial m}{\partial t}\right\rfloor_w-(u_j-w_j)\frac{\partial m}{\partial x_j}=0$$

$$\frac{{u_i}^{n+1}-{u_i}^n}{\Delta t}-\frac{{F_i}^{n+1/2}}{m^n}-\frac{1}{\Delta t m^{n+1}}\sum_f(\rho u_i)^*\,\delta V^*=0 \quad\Longleftrightarrow\quad \rho\left\lfloor\frac{\partial u_i}{\partial t}\right\rfloor_w+\frac{\partial p}{\partial x_i}-\rho(u_j-w_j)\frac{\partial u_i}{\partial x_j}=0$$

$$\frac{e^{n+1}-e^n}{\Delta t}-\frac{{F_i}^{n+1/2}}{2m^n}({u_i}^*+{u_i}^n)-\frac{1}{\Delta t m^{n+1}}\sum_f(\rho e)^*\,\delta V^*=0 \qquad \rho\left\lfloor\frac{\partial e}{\partial t}\right\rfloor_w+p\frac{\partial u_i}{\partial x_i}-\rho(u_j-w_j)\frac{\partial e}{\partial x_j}=0$$

and recall that for face f, $\delta V=\Delta t(u_j-w_j)A_j$

An operator splitting error results from the use of post-Lagrange values in the remap step and will be *O(Δt)* accurate unless Strang splitting is used

The remap step in this form is easily shown to be 1st-order accurate in time

- Begin with the Lagrange-ALE mass equation and integrate over a control volume (which gives an equation for zone *z*):

$$\int \frac{1}{V}\left[\frac{\partial m}{\partial t}\right]_w dV = \left[\frac{\partial m_z}{\partial t}\right]_w$$

$$\int \frac{1}{V}(u_j - w_j)\frac{\partial m}{\partial x_j} dV = \int \frac{1}{V}(u_j - w_j) m dA_j = \sum_f \rho\,(u_j - w_j)A_j$$

- Discretizing the time derivative with forward Euler and combining terms gives

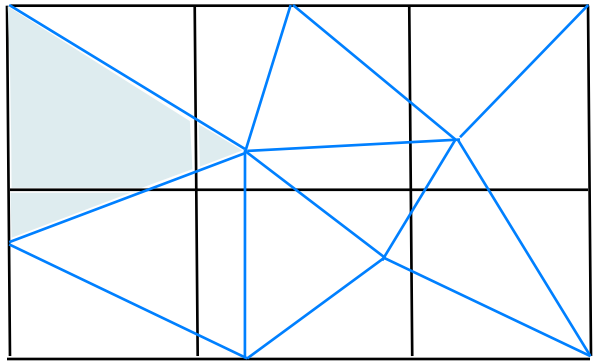
$$\frac{m^{n+1} - m^n}{\Delta t} = \sum_f \left[\rho(u_j - w_j)A_j\right]^n = \frac{1}{\Delta t}\sum_f [\rho \delta V]^n$$

which is exactly the remap step but with * replaced by n. The analysis is easily repeated for the remaining equations.

The standard remap procedure is equivalent to a forward Euler method and will be *O(Δt)* accurate unless a higher accuracy time integration method is used.

What about the discontinuous remap (*i.e.* mesh-mesh intersection) method?

- Obviously the analysis is more complicated since a given zone may not exist from one time step to the next
- However, the intersection process still computes δV for a set of fluid elements from one time step to the next
  (we've just allowed for the possibility that the initial or final volume of a zone can be zero)



- Our *hypothesis*, therefore, is that the discontinuous remap method will also show 1st-order accuracy in time

Note that if the remap step did not affect time accuracy, we would not expect the use of a remap step to affect temporal convergence rates!

Numerical experiments were performed to test our hypotheses

- Experiment: measure self-convergence with decreasing time step relative to a fine time step result on a fixed spatial mesh
- 1D Test problems (see JCP article for definitions):
  - Smooth flow problem (Kenamond & McAbee)
  - Shock Tube
- Methods:
  - Pure Lagrange with 1st or 2nd order Runge-Kutta (RK) integration
  - Lagrange plus remap with Lie or Strang splitting and RK1 or RK2 for remap terms
  - Unsplit method with RK2
  - Discontinuous remap method (DRM)
  - Test both donor cell (1st order) and piecewise linear (2nd order) advection schemes

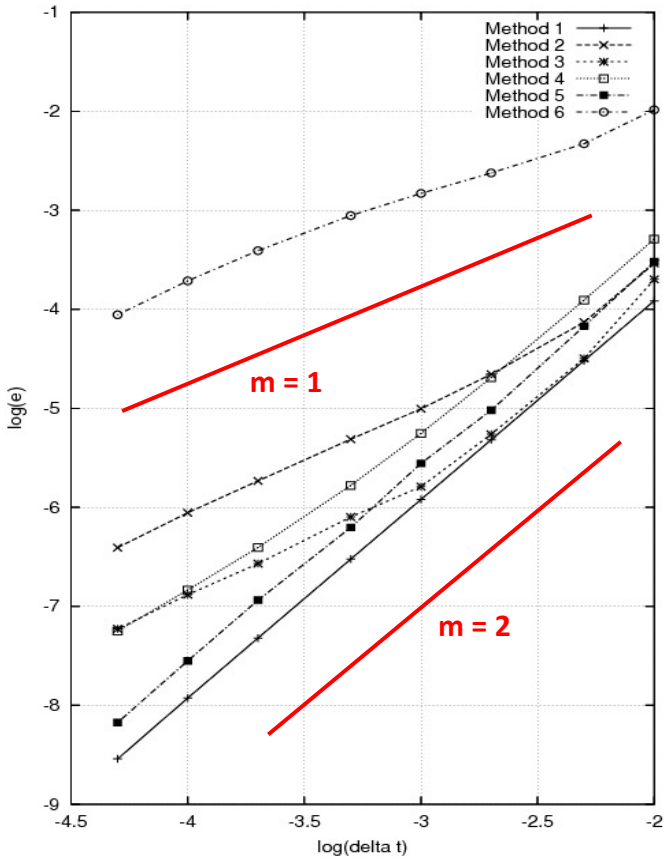
While it is true that Δx and Δt are related in hyperbolic problems, reality is not that simple

- The Courant condition is a stability constraint, not an accuracy constraint
  - A given set of stable methods will not necessarily have the same accuracy
- Many codes must run at a Courant number well below 1.0
  - Increasing time accuracy often allows the Courant number to be increased
- The Courant condition is not always the limiting factor
  - We have observed mesh tangling at sub-Courant time steps that does not occur if the time step is decreased or time accuracy is increased
- In highly nonlinear problems, small errors compound
  - For example, in a burning DT plasma, the reaction rate scales as $\rho^2 T^4$
- Varying Δt at fixed Δx is actually how most production codes are run
  - Users pick a resolution they can afford and vary the time step controls as needed

Temporal convergence studies at fixed mesh size allow time accuracy to be quantified in isolation from spatial operators.

Results for the smooth flow problem are consistent with our hypotheses

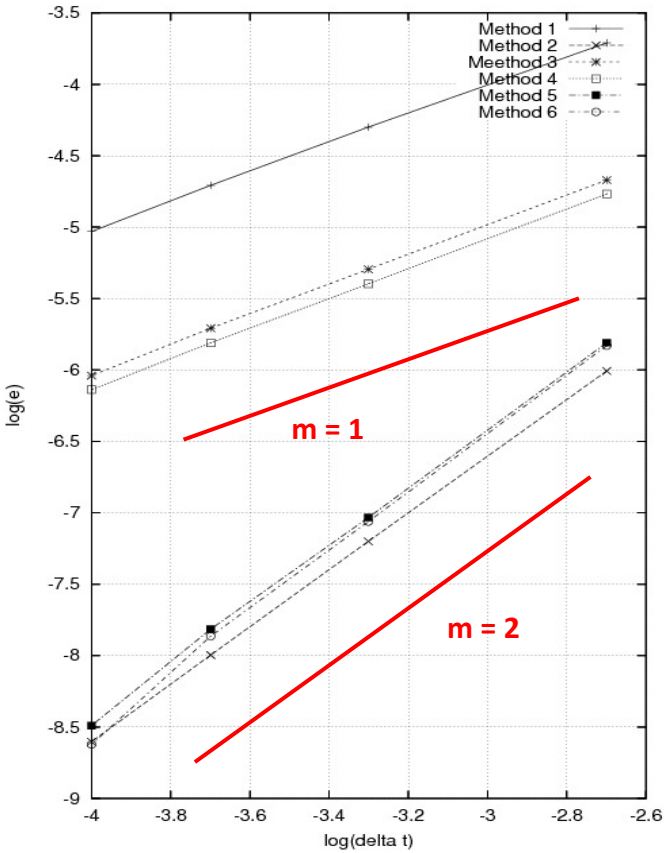
- Methods and average convergence rate:
  1. RK2 Lagrange: 2.0
  2. RK2 Lagrange + Lie/RK1 remap: 1.2
  3. RK2 Lagrange + Strang/RK1 remap: 1.5
  4. RK2 Lagrange + Strang/RK2 remap: 1.7
  5. Unsplit RK2: 2.0
  6. RK2 Lagrange + DRM: 0.92
- ALE methods undo half the Lagrange displacement at each time step
- The DRM used a piecewise linear reconstruction (PLR); all other advection schemes used donor cell (DC)



Although the use of Strang splitting and an RK2 remap improves accuracy, only the unsplit method matches the 2nd-order convergence of the RK2 Lagrange method.

Results for the shock tube problem are consistent with our hypotheses (using a point in the nonlinear expansion fan)

- Methods and average slope:
  1. RK1 Lagrange: 1.02
  2. RK2 Lagrange: 2.0
  3. RK2 Lagrange + Lie/RK1 remap (DC): 1.05
  4. RK2 Lagrange + Lie/RK1 remap (PLR): 1.06
  5. RK2 Unsplit (DC): 2.08
  6. RK2 Unsplit (PLR): 2.09
- Methods 3 & 4, and 5 & 6, use identical time integration but different advection schemes



Only the unsplit method matches the 2nd order convergence of the RK2 Lagrange method. The advection scheme does not change the convergence rate.

Based (in part) on these studies we have implemented unsplit ALE in our 3D unstructured mesh code CHICOMA

- CHICOMA solves the flux-conservative ALE equations on tetrahedral meshes with AMR

$$\frac{1}{V}\frac{\partial}{\partial t}\left[V\begin{pmatrix}\rho\\ \rho u_i\\ \rho E\end{pmatrix}\right]_w + \frac{\partial}{\partial x_j}\begin{bmatrix}\rho(u_j - w_j)\\ \rho u_i(u_j - w_j) + p\\ \rho E(u_j - w_j) + p u_j\end{bmatrix} = \begin{bmatrix}S_\rho\\ S_{u,i}\\ S_E\end{bmatrix} \qquad E = e + \frac{1}{2}u_i u_i$$

- Spatial scheme: Edge-based FE scheme for linear tetrahedra (node-centered)
- Time integration: Explicit multi-stage RK scheme with unsplit mesh motion
- The choice of flux and mesh velocity determine the method
  - Eulerian: $w_j = 0$, Rusanov or HLLC flux, parabolic MUSCL reconstruction
  - Lagrangian: $w_j = u_j$, Morgan-Waltz-Burton "flux", optional TTS-like model
  - ALE mode: Eulerian or Lagrangian solver + mesh velocity option

This approach provides a consistent numerical framework for Eulerian, Lagrangian, and ALE algorithms in the same code, with AMR.

The mesh velocity is initially set to the fluid velocity, and then smoothed to mitigate tangling

- The linear system

$$k\nabla^2 w_i = 0$$

  is solved to some specified tolerance ϵ_w
- The diffusion coefficient at each node is given by

$$k = c_1 max\left(0{,}1 - c_2 \frac{\|\omega_i\|}{\|\omega_i\|_\infty}\right)$$

  where c_1 and c_2 are input parameters.
- This form allows regions of high vorticity to be treated more Eulerian-like, and regions of low vorticity to be treated more Lagrangian-like

This scheme allows the mesh to follow the flow in a robust manner. Mesh motion will occur only where the fluid velocity is nonzero!

Our method satisfies the Geometric Conservation Law to truncation error

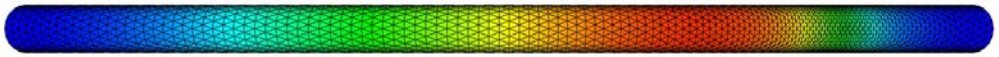
- Geometric conservation law: $\frac{1}{V}\frac{\partial V}{\partial t} = \frac{\partial w_i}{\partial x_i}$
- Test problem:
  - Uniform density field on shock tube mesh with mesh velocity given by

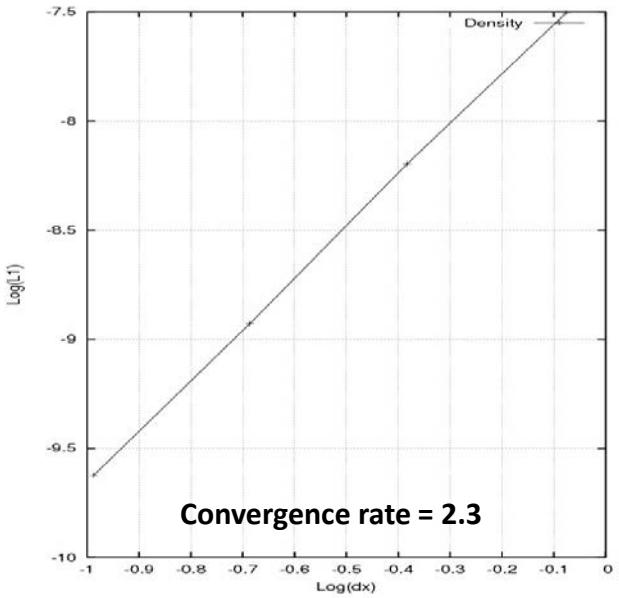
$$w_z = sin^2 \frac{\pi z}{100}$$

  - Evolve for 20 time units and measure error relative to exact uniform solution

Time = 0.000

Time = 20.000

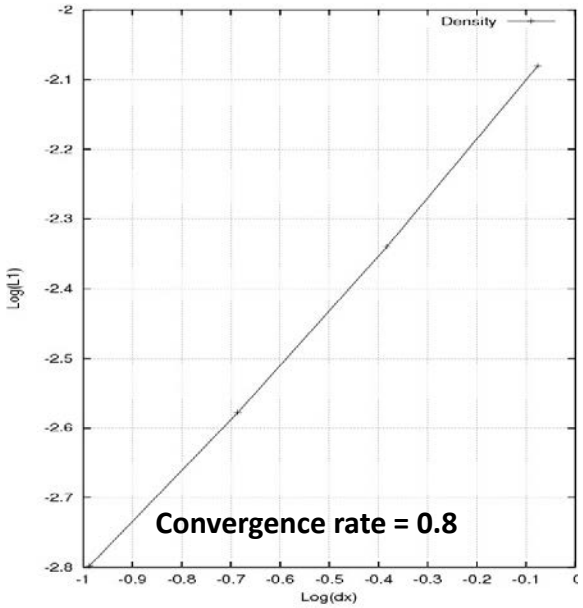


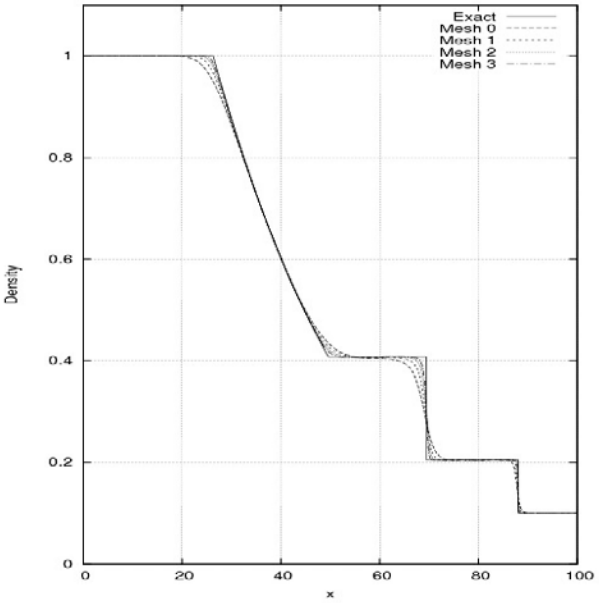


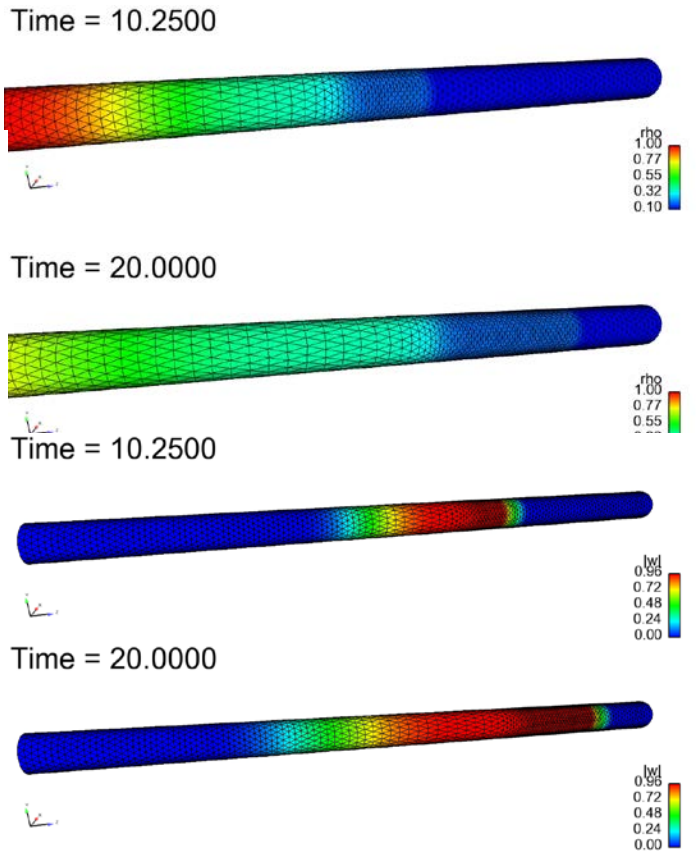
Mesh	Points	Tets	Ave. dx
0	7294	34181	0.840
1	51794	273448	0.414
2	389139	2187584	0.206
3	2014277	17500672	0.103

The method exhibits 1st-order spatial accuracy on a shock tube problem

- Order of magnitude pressure/density ratio across interface
- Same set of meshes used for GCL problem
- Error measured along centerline of 3D mesh





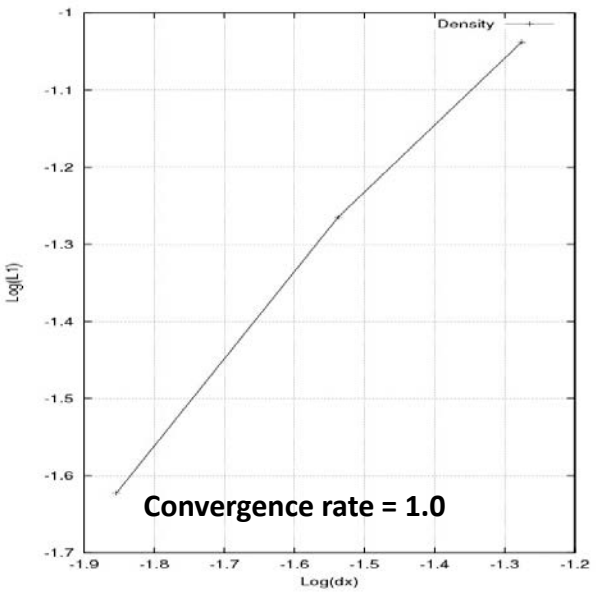


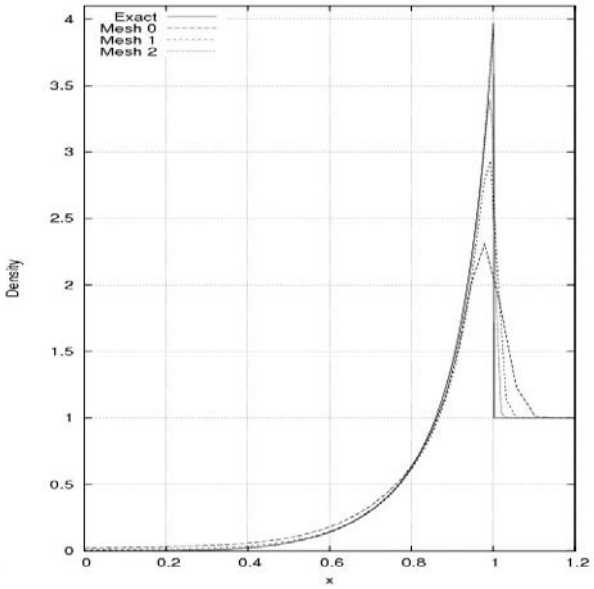
$c_1 = 1.0, c_2 = 0, \epsilon_w = 0.5$

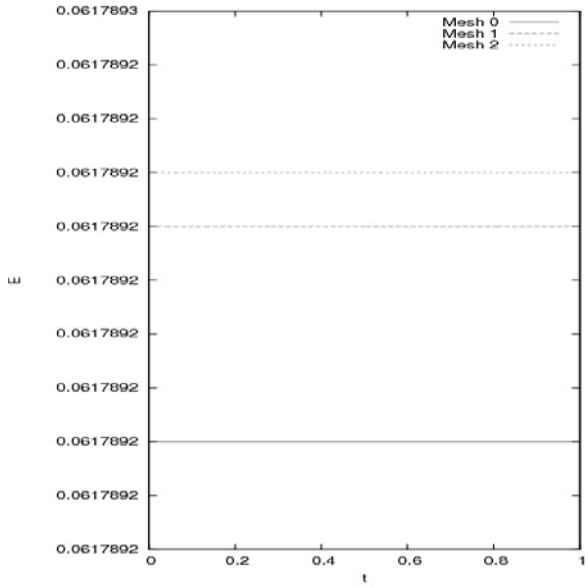
The method exhibits 1st-order spatial accuracy on the Sedov problem

- Standard Sedov definition
- Error measured along x-axis
- Total energy is conserved exactly

Mesh	Points	Tets	Ave. dx
0	7294	34181	0.840
1	51794	273448	0.414
2	389139	2187584	0.206



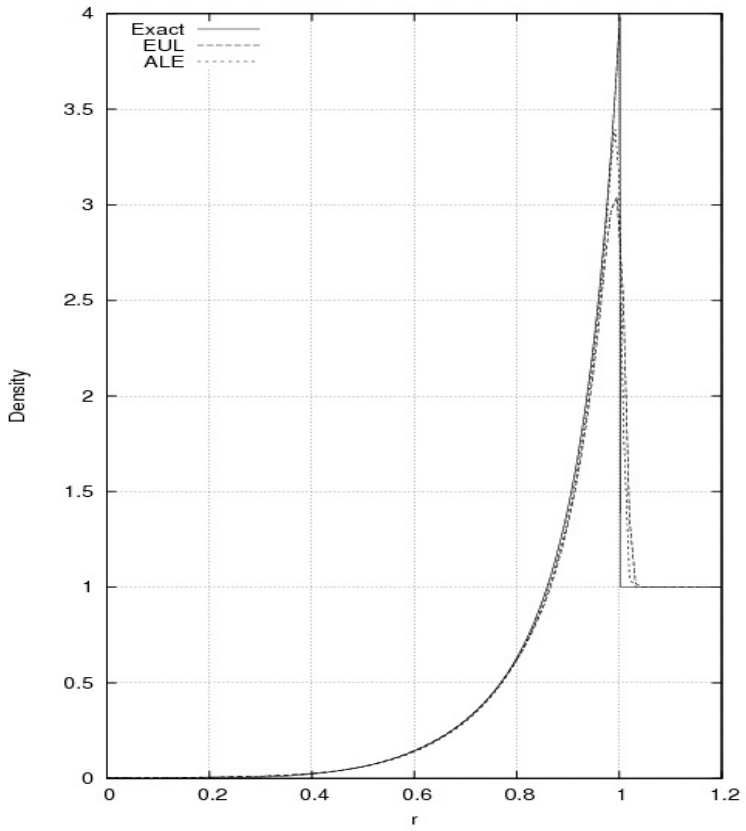


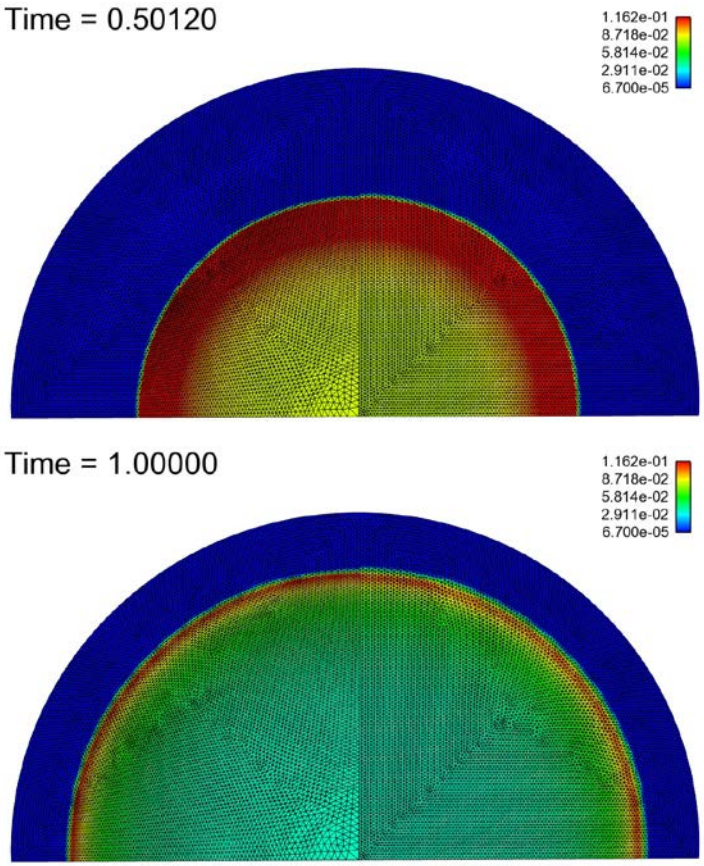


$c_1 = 0.5, c_2 = 0, \epsilon_w = 0.25$

ALE increases peak density by 10% over a direct Eulerian solution on the finest mesh

- Higher density results from smaller mesh size near shock

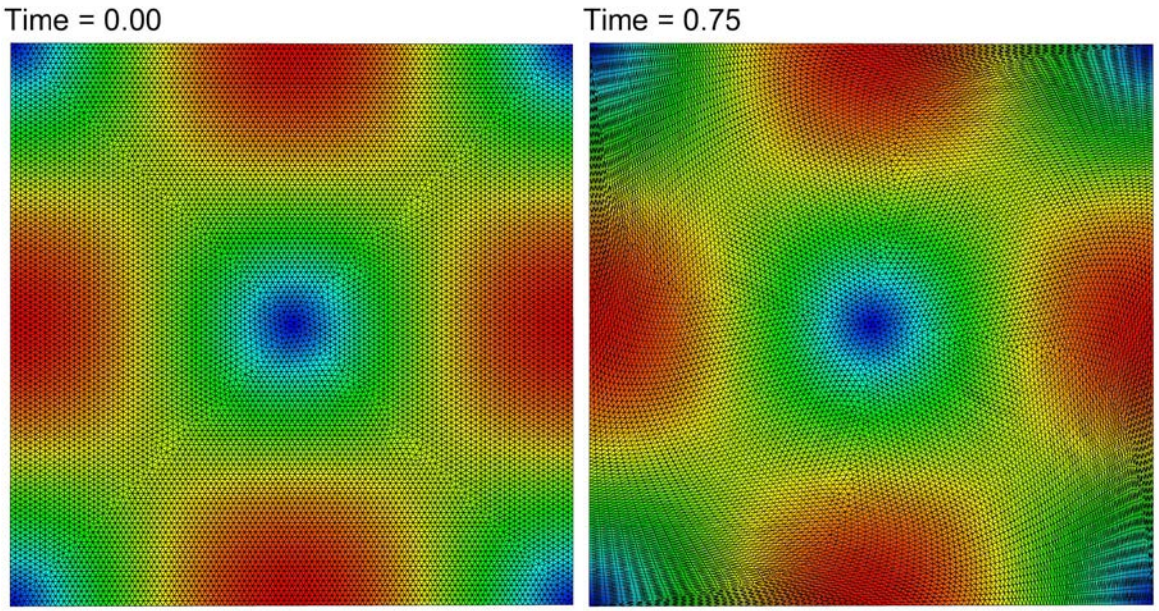


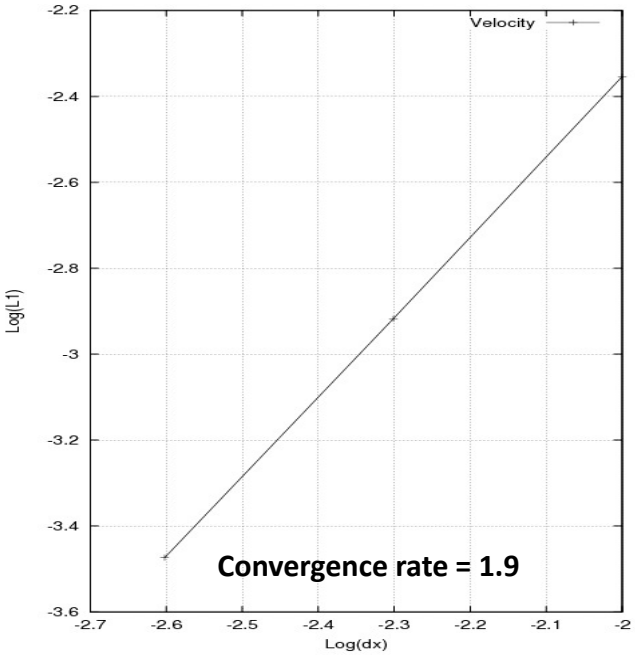


The method exhibits 2nd-order spatial accuracy on the Taylor-Green problem

- Run as steady state problem with source term
- Two zones thick in z-direction on coarsest mesh

Mesh	Points	Tets	Ave. dx
0	24530	75912	0.011
1	148378	607296	0.0055
2	997679	4858368	0.0028

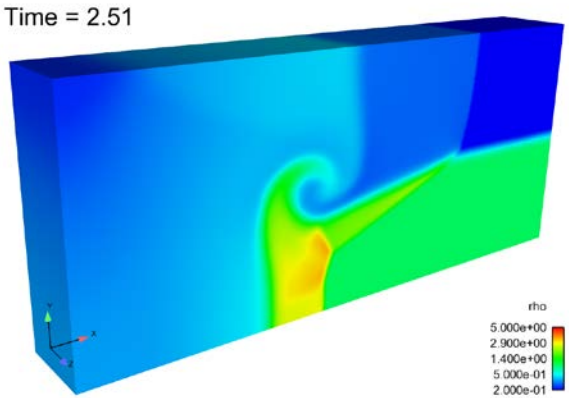


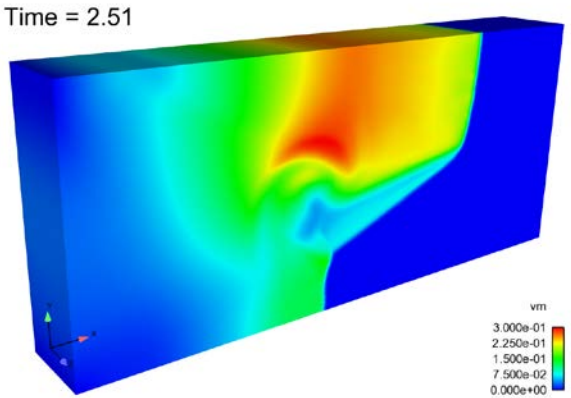


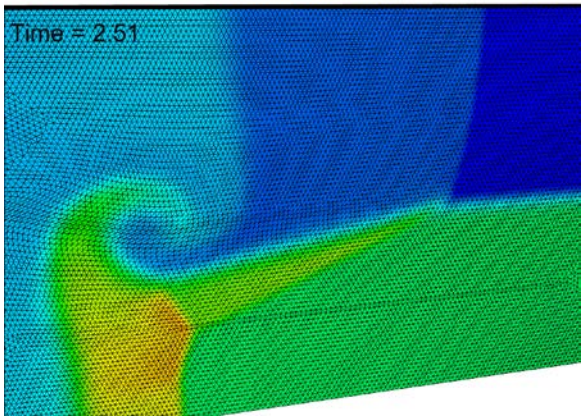
$c_1 = 0.5, c_2 = 0.5, \epsilon_w = 0.2$

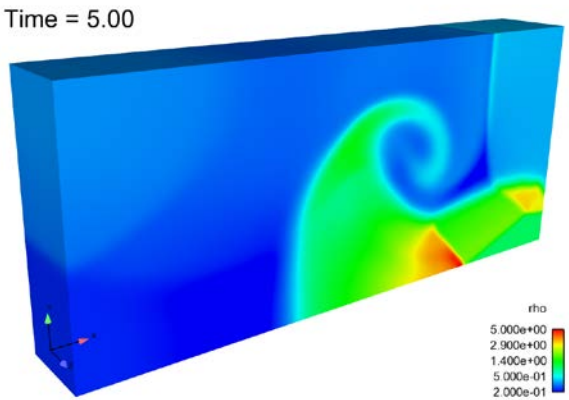
The mesh motion algorithm is robust on a single-material variant of the triple point problem

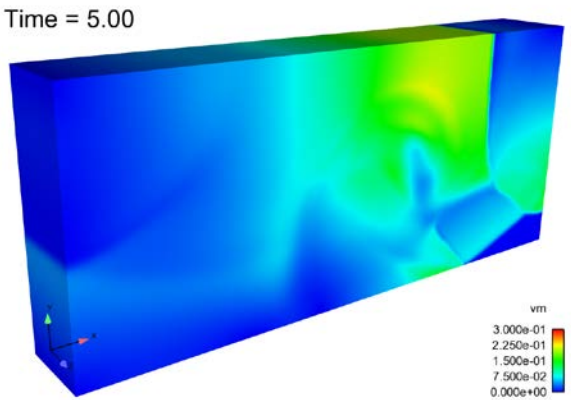
- Mesh of 2 x 10^6 tetrahedra

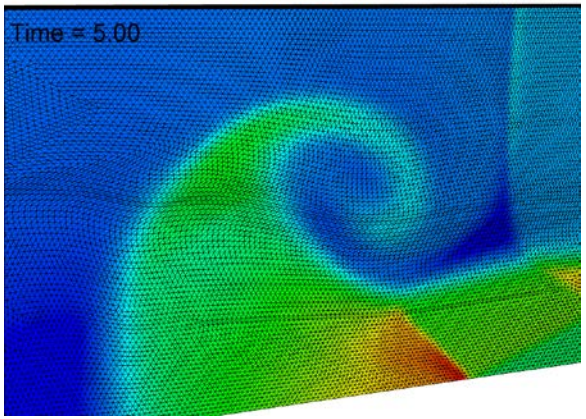












$c_1 = 0.25$, $c_2 = 0.5$, $\epsilon_w = 0.2$

The time accuracy characteristics of the Lagrange-plus-remap ALE method have been investigated

- The standard Lagrange-plus-remap method is shown, both analytically and numerically, to be 1st-order accurate in time
  - Errors result from operator splitting and low-order time integration of remap terms
  - Errors exist even if the underlying Lagrange step is 2nd-order accurate in time
- A 2nd-order accurate (in time) ALE method can be achieved with an *unsplit* treatment of the remap terms
  - Improvements to the Lagrange-plus-remap method also are possible
- Application of unsplit ALE to 3D shock hydrodynamics is demonstrated on unstructured meshes of up to 10^7 tetrahedra
  - The method satisfies the Geometric Conservation Law to truncation error
  - Convergence under mesh refinement is observed at the expected order of accuracy

References

1. J. Waltz, N.R. Morgan, T.R. Canfield, M.R.J. Charest, L.D. Risinger, and J.G. Wohlbier, `A three-dimensional finite element arbitrary Lagrangian-Eulerian method for shock hydrodynamics on unstructured grids', LANL report no. LA-UR-13-25216, submitted to Comput. Fluids (2013).
2. J. Waltz, `Operator splitting and time accuracy in Lagrange plus remap solution methods', J. Comput. Phys. 253:247-258 (2013).
3. J. Waltz, T.R. Canfield, N.R. Morgan, L.D. Risinger, and J.G. Wohlbier, `Verification of a three-dimensional unstructured finite element method using analytic and manufactured solutions', Comput. Fluids 81:57-67 (2013).