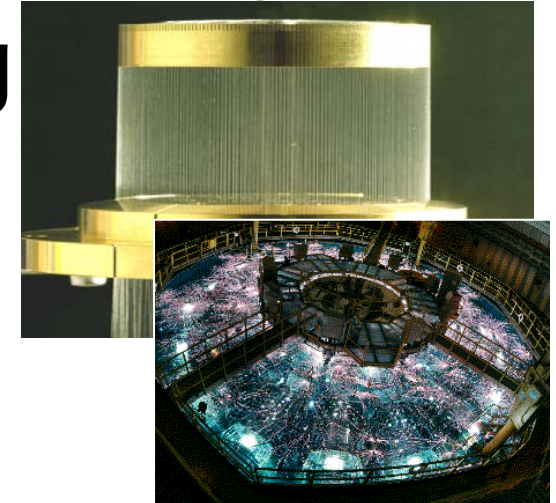
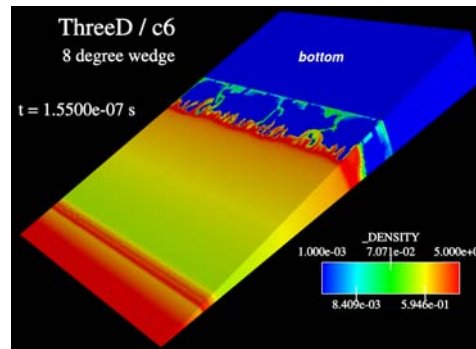
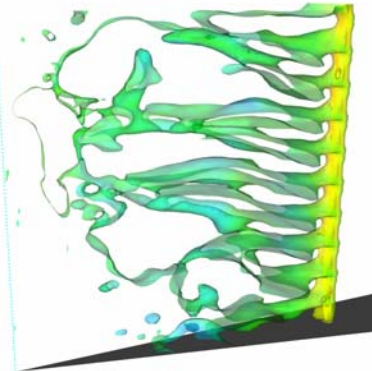
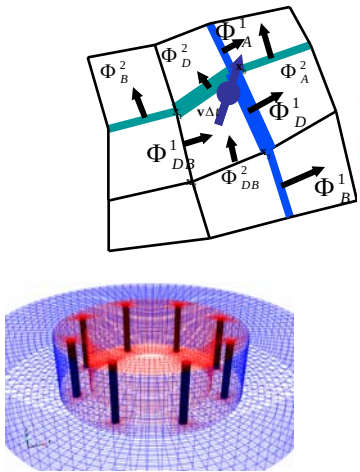




Algorithm Developments in Alegra Guided by Testing



W. Rider, **A. Robinson**, G. Weirs, C. Ober, E. Love, H. Hanshaw, R. Lemke,
G. Scovazzi, J. Shadid, J. Banks
Sandia National Laboratories, Albuquerque, NM

Numerical methods for multi-material fluid flows
Czech Technical University, Prague, Czech Republic
September 10 - 14, 2007



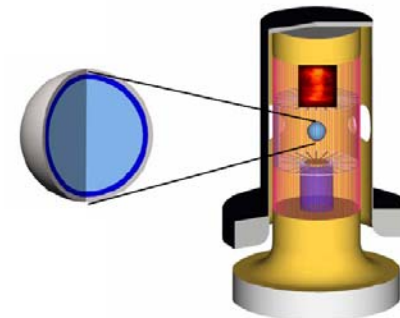
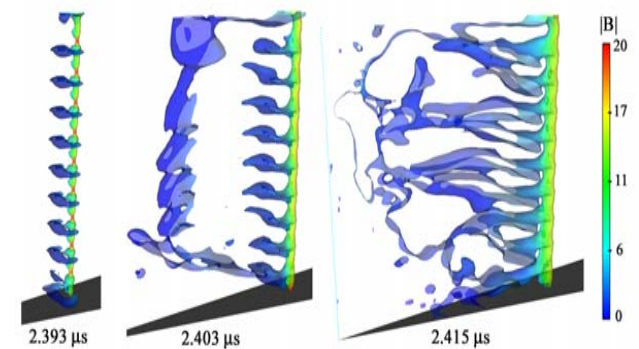
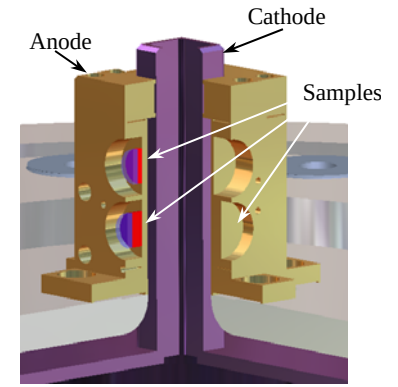
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL84000.





Talk Outline

- Alegria application focus
- Algorithm development areas:
 - Lagrangian hydro
 - Remap methods
 - Eulerian frame hydro
- Application performance improvements
- Future directions





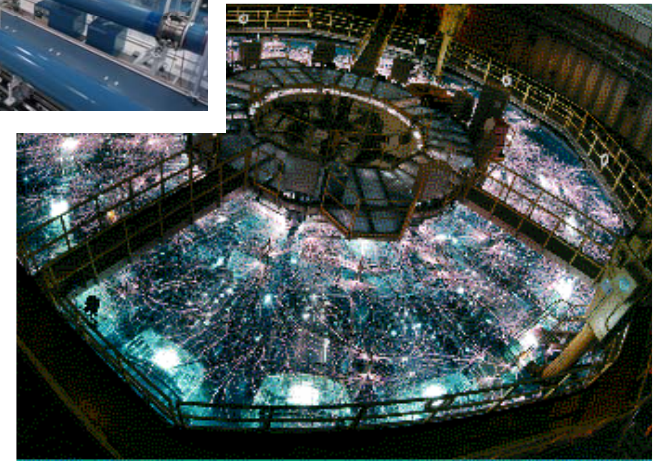
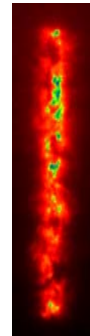
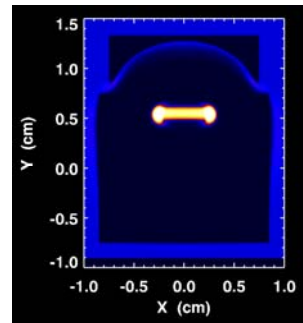
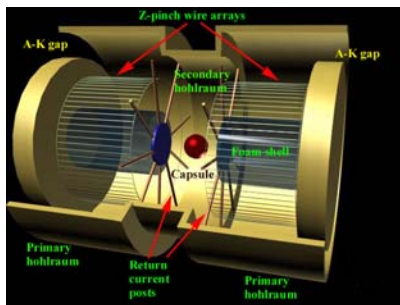
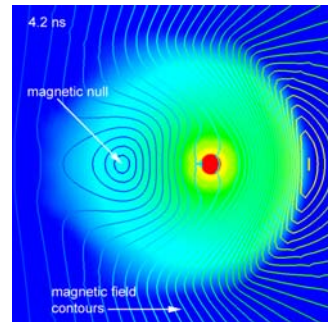
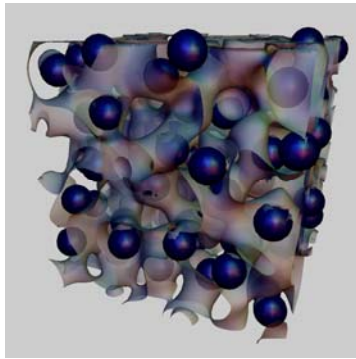
Introduction to Alegra

- Alegra began in 1990 with the object of producing an advanced ALE code
- The code has shock hydrodynamics with resistive MHD, radiation transport,...
 - Uses standard hydro & remap methods (need improvement)
 - Advanced resistive MHD, linear algebra, constitutive models



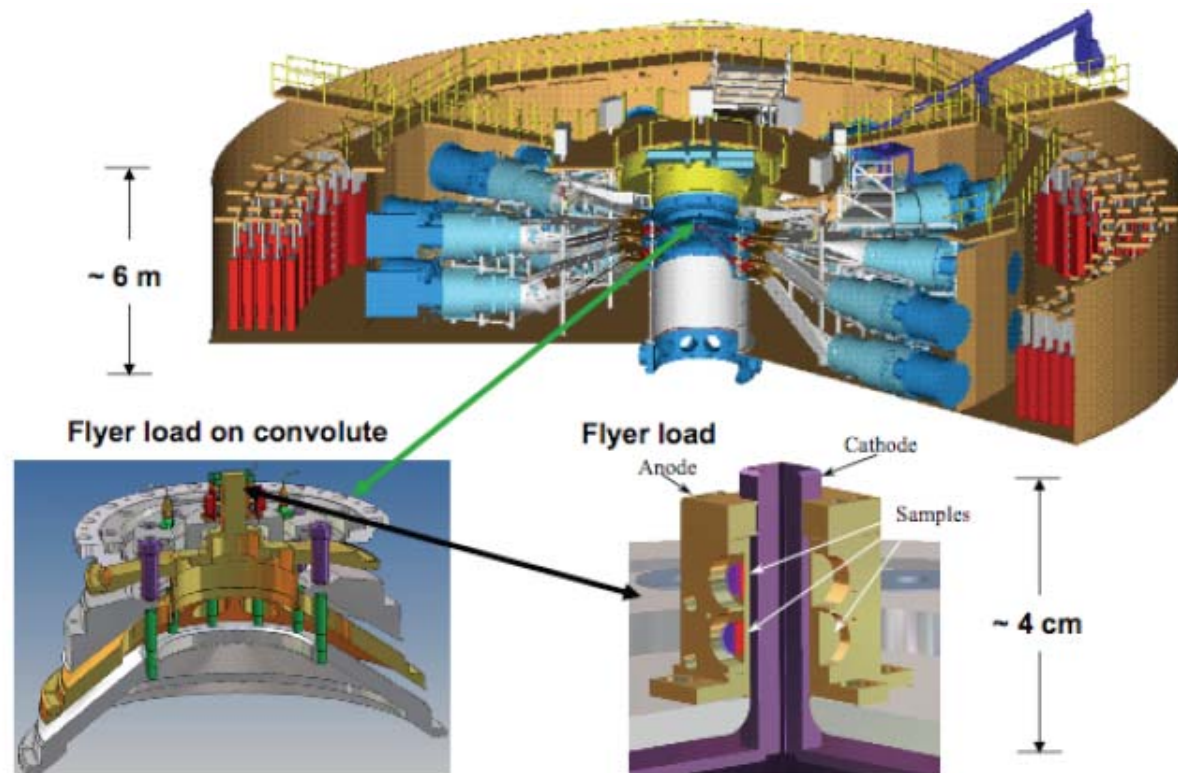
Alegra Application - HEDP

- One of the key applications for Alegra is high energy density physics at Z.



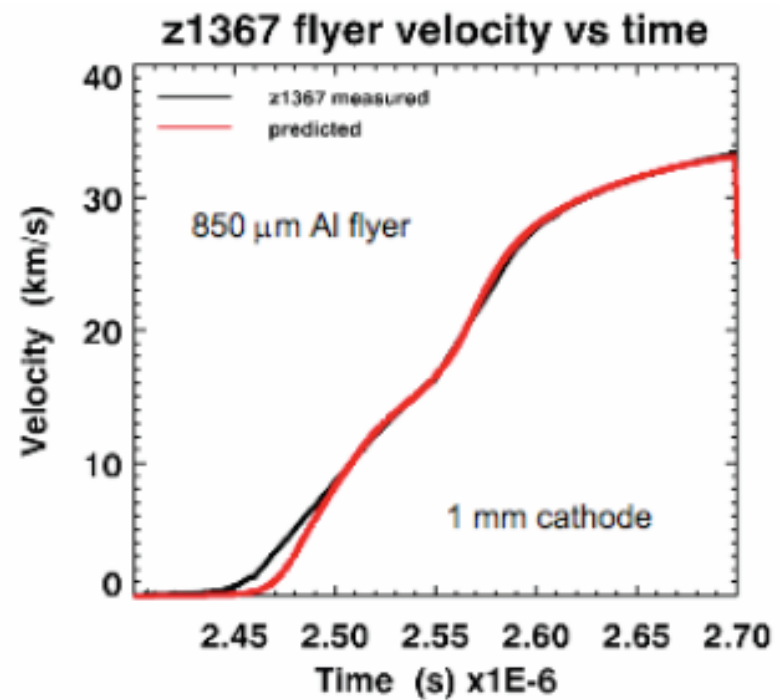
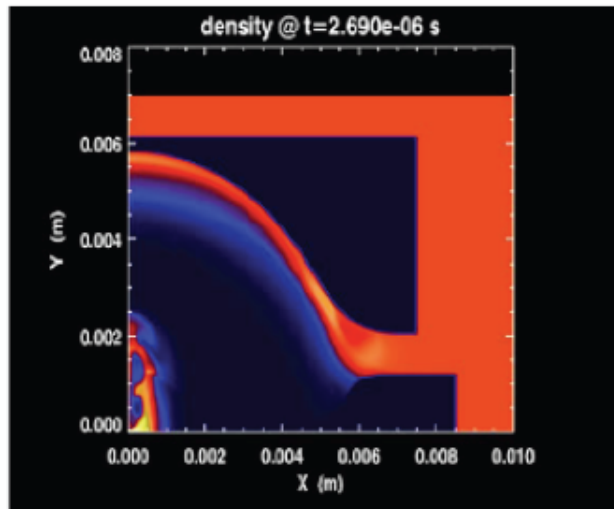
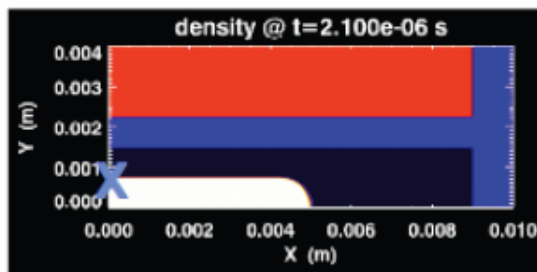


Z-Machine is a great testbed for multiphysics





Fantastic Results with Flyer Plates.





Algorithm/process challenges still exist

- We focus on the areas where the algorithms are “*standard*,” but not *state-of-the-art*.
 - Hydrodynamics
 - Lagrangian hydrodynamics
 - Remap
 - Eulerian
- } Testing is a primary focus with response leading to improvement
- Sustainable verification processes must be implemented alongside testing and improvement processes.
 - Identify useful problems
 - Install problems in a permanent repository in a state which permits future testing in as automated a way as possible.

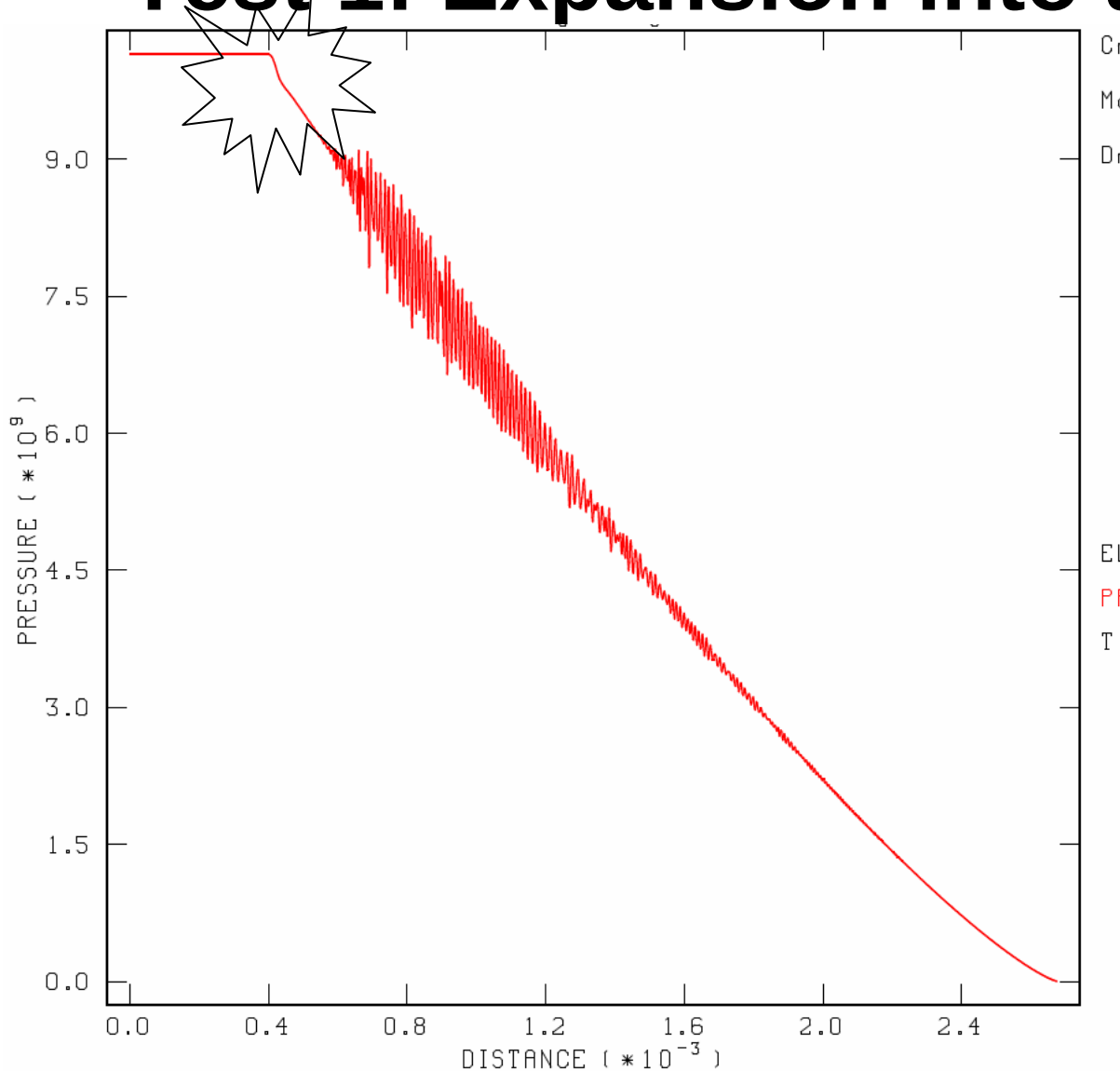


Lagrangian Hydro development is critical.

- **The Lagrangian hydro algorithm in Alegra is based on the method from (SNL code) Pronto.**
- **It uses the Von Neumann-Richtmyer time-space staggering, but the energy equation is first-order in time; however the method is conservative.**
 - **It's the “same” as the predictor in the compatible P-C method, except for the time-centering.**
- **Full stability analysis for this method was not available (except for Hicks '77).**



Test 1: Expansion into a vacuum



- Results from expansion problem: instability is seen at high resolution and long times
- Seen sooner in applications
- Conservative but unstable.



Stability analysis of the Alegra Lagrangian Hydro method

- First write the equations in 1-D (w/o Q)

$$x_{j+1/2}^{n+1} = x_{j+1/2}^n + \Delta t u_{j+1/2}^{n+1/2} \quad \equiv \quad \frac{V_j^{n+1} - V_j^n}{\Delta t} - \frac{u_{j+1/2}^{n+1/2} - u_{j-1/2}^{n+1/2}}{m_j} = 0$$

$$\frac{u_{j+1/2}^{n+1/2} - u_{j-1/2}^{n+1/2}}{\Delta t} + \left(\frac{p_{j+1}^n - p_j^n}{m_{j+1/2}} \right) = 0 \quad \frac{e_j^{n+1} - e_j^n}{\Delta t} + p_j^n \left(\frac{u_{j+1/2}^n - u_{j-1/2}^n}{m_j} \right) = 0$$

$$p = (\gamma - 1) e / V$$

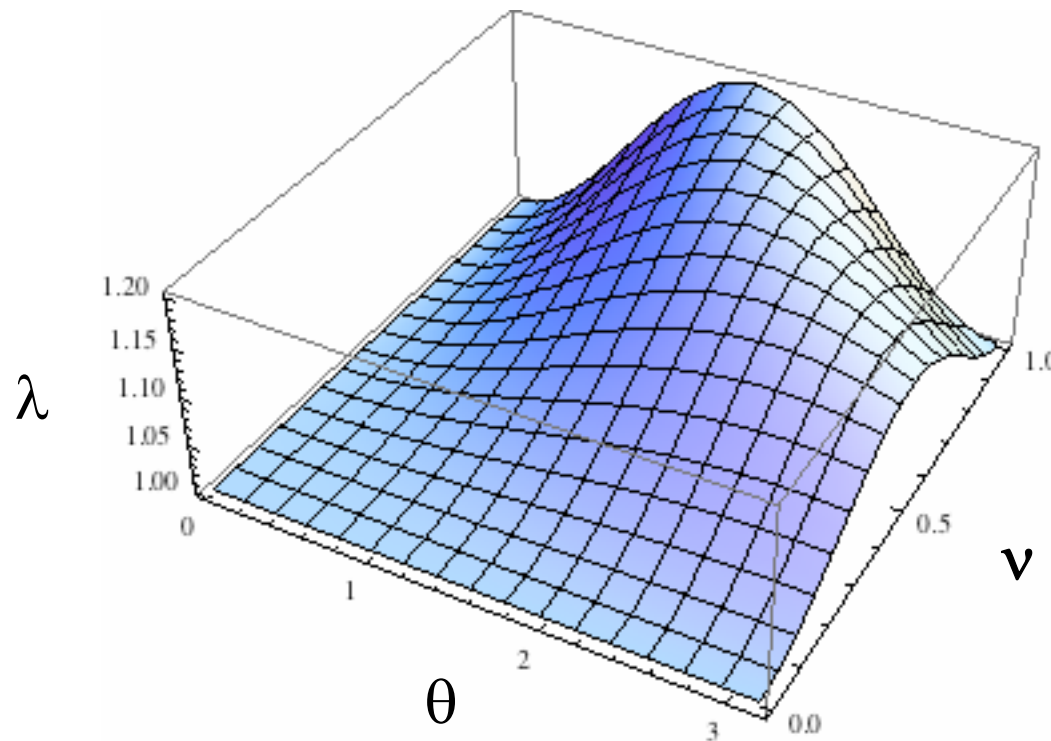
$\uparrow$
 $u_{j+1/2}^n = \frac{u_{j+1/2}^{n+1/2} + u_{j+1/2}^{n-1/2}}{2}$

- Linearize, apply the Fourier transform and find the diagonal of the “Jacobian”



Examine the eigenvalues of the system

- Two of the eigenvalues are OK, one is a problem,

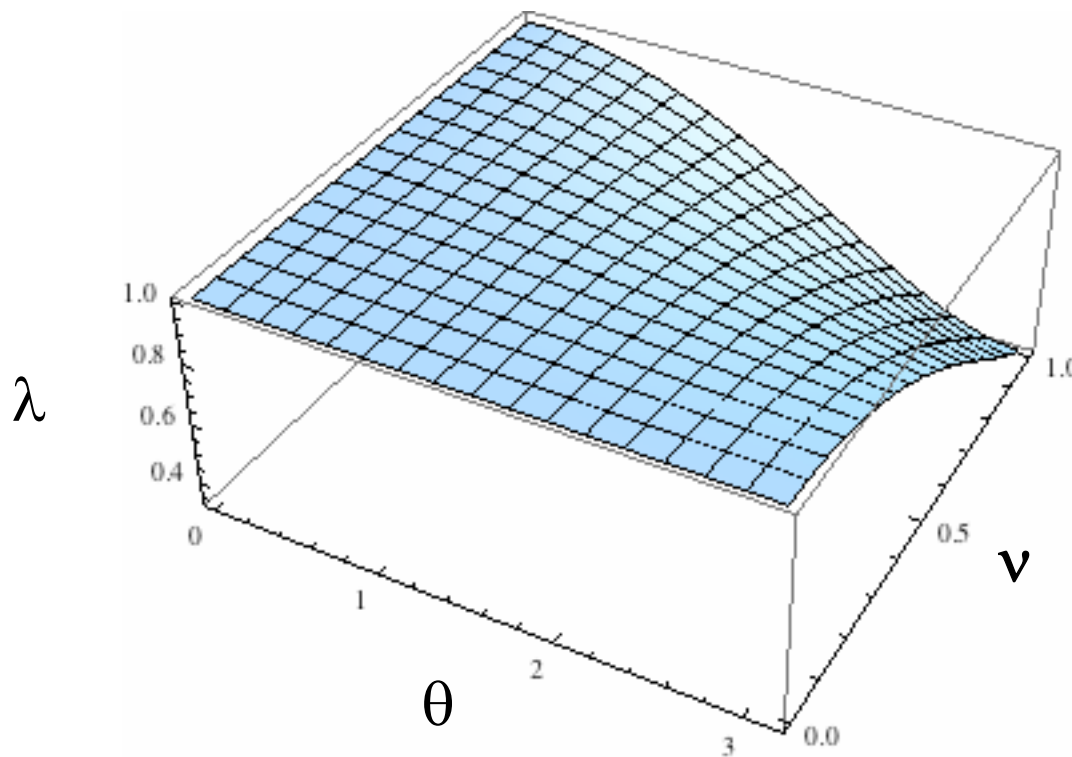


**Mach number
 $u/c = 1$**



This eigenvalue can be stabilized by using artificial viscosity.

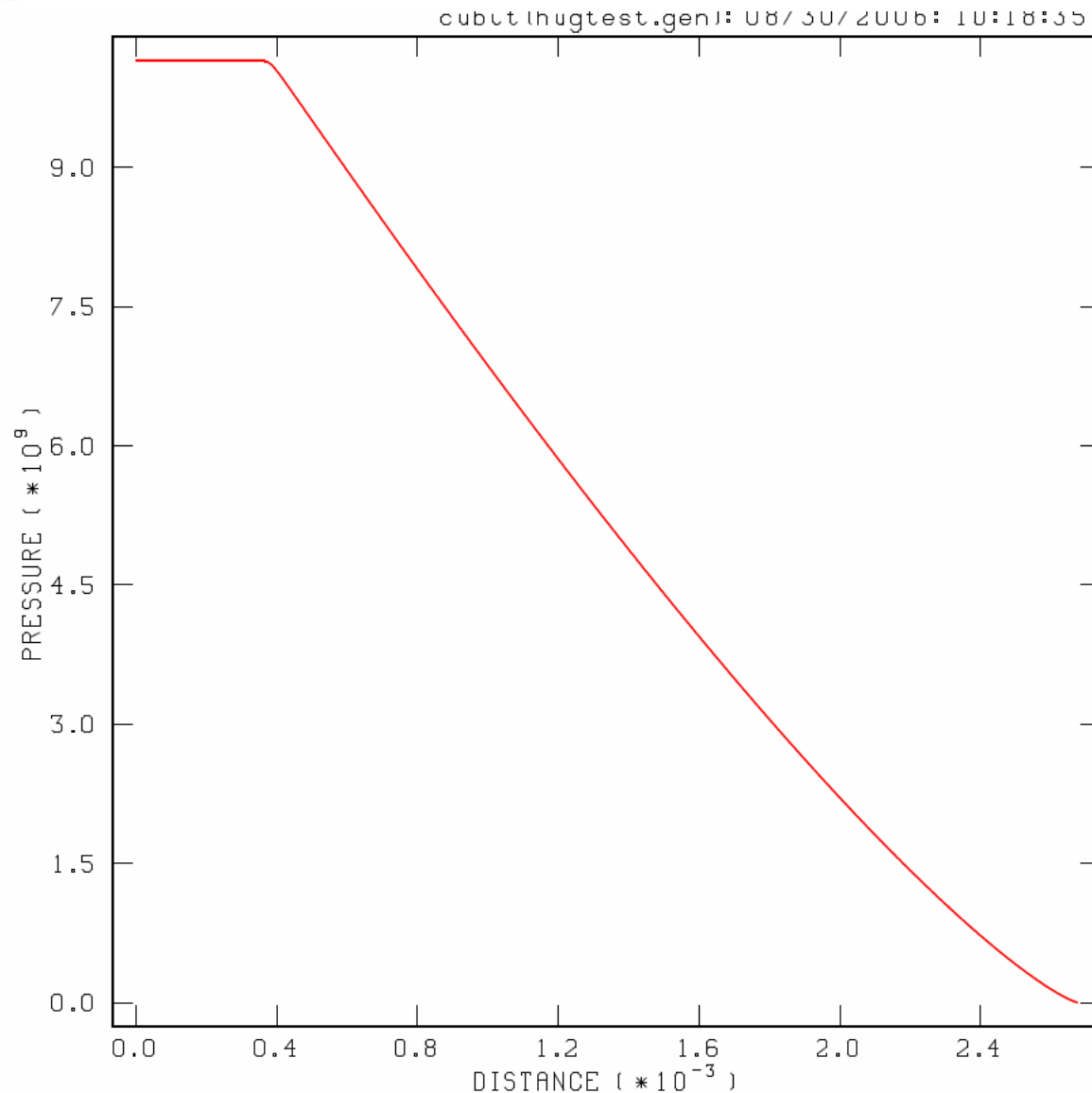
- **Examine the eigenvalue with a linear Q**



**Mach number
 $u/c = 1$**



The expansion can be stabilized in several ways.



Change discrete energy equation -> lose conservation

Add viscosity -> loss of isentropic behavior

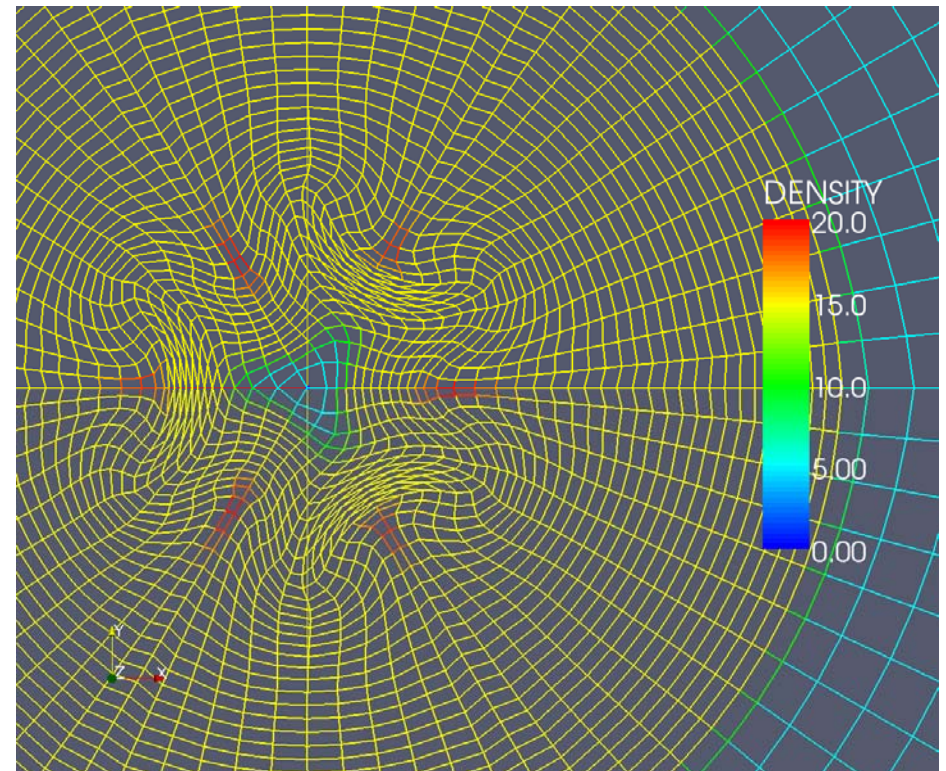
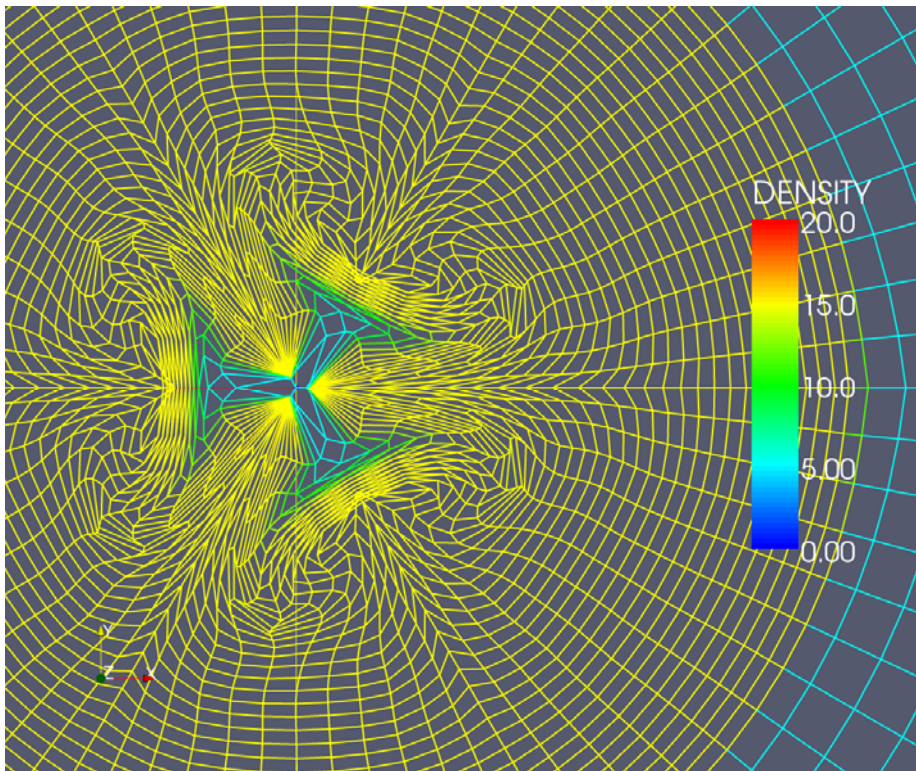
Results of either fix “looks” the same.

Neither is optimal, begs in the long term to do stable and conservative solution.



Tensor viscosity results

We examine the performance of the code on the “trisection” mesh, left is the old Q, right is the same problem with the new tensor Q. It uses Noh’s shock reflection in 2-D.





Remesh and Remap

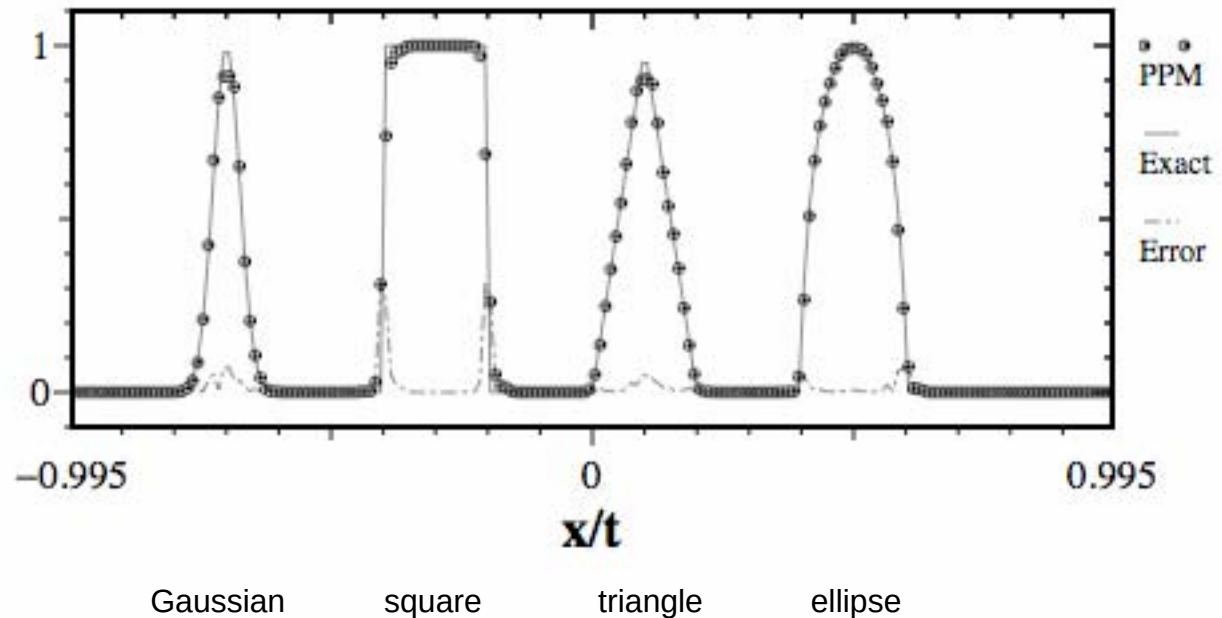
- The remesh has recently been extensively overhauled by Tom Voth.
- The remap has been the focus of several developments.
 - The change with the most impact from an application's point-of-view is the implementation of the DeBar kinetic energy advection.
 - Remap differencing is also being carefully tested and evaluated (next slide).
 - The differencing is being enhanced for accuracy on uneven meshes.
 - Enhanced interface reconstruction developed by Jay Mosso (See other talk this conference.)



Start with the simple stuff - linear advection

- Solved a simple multi-pulse advection

200
cells



- Found a bug in the superbee limiter (square wave problem is enough)

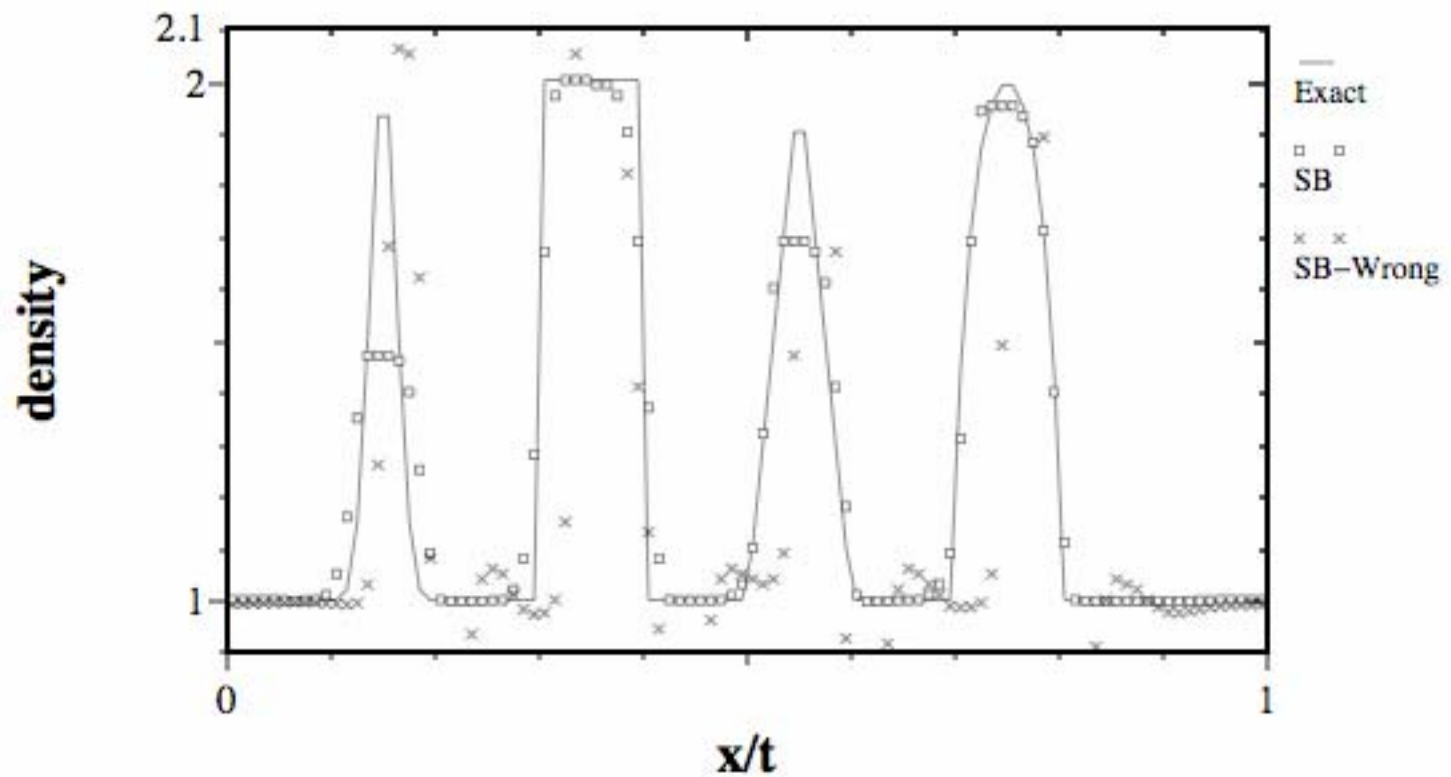


Even simple testing is necessary

- **Superbee limiter error - subtle!**

$$s_j = \min \text{mod} \left[4, 4r, \max \text{mod}(1, r) \right] \frac{\Delta u}{\Delta x} \quad \Rightarrow \quad s_j = \min \text{mod} [2, 2r, \max \text{mod}(1, r)] \frac{\Delta u}{\Delta x}$$

100
cells





Our implementation of the “DeBar fix” for conserving energy in remap.

- This is a modern implementation of DeBar’s kinetic energy treatment.

$$KE = \frac{1}{nodes} \sum_{nodes} \frac{1}{2} \mathbf{u}^2$$

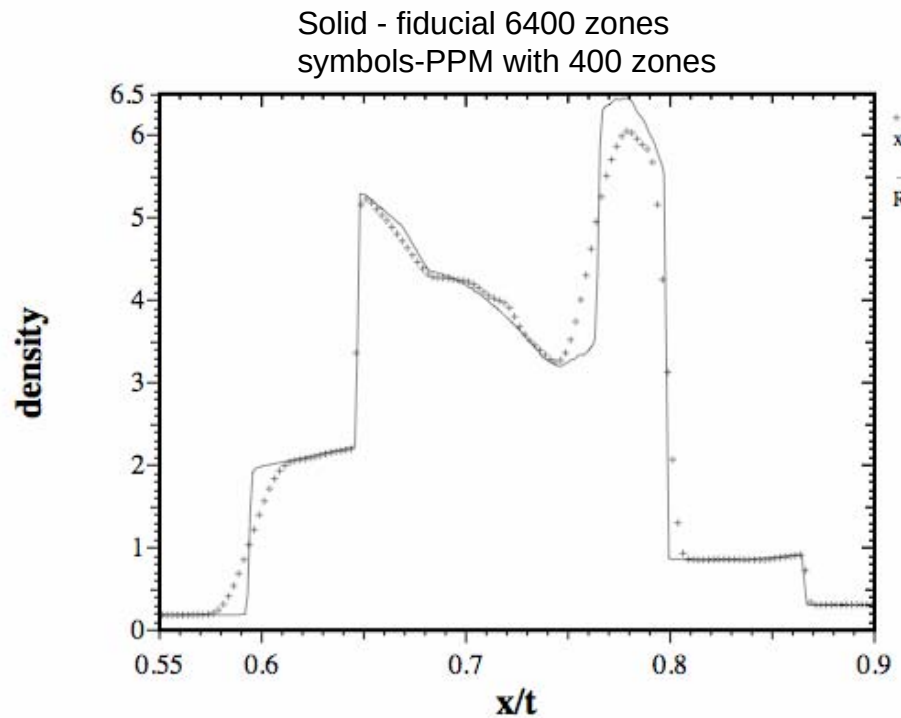
$$\rho e = \rho e + (KE_{remapped} - \frac{1}{nodes} \sum_{nodes} \frac{1}{2} \mathbf{u}^2_{remapped})$$

- It corrects for the process of remap on the kinetic energy and allows full conservation of energy.
- We use a Q/p > 0.001 switch to avoid using the fix away from shocks.
- This approach will also be implemented for magnetic field energy.

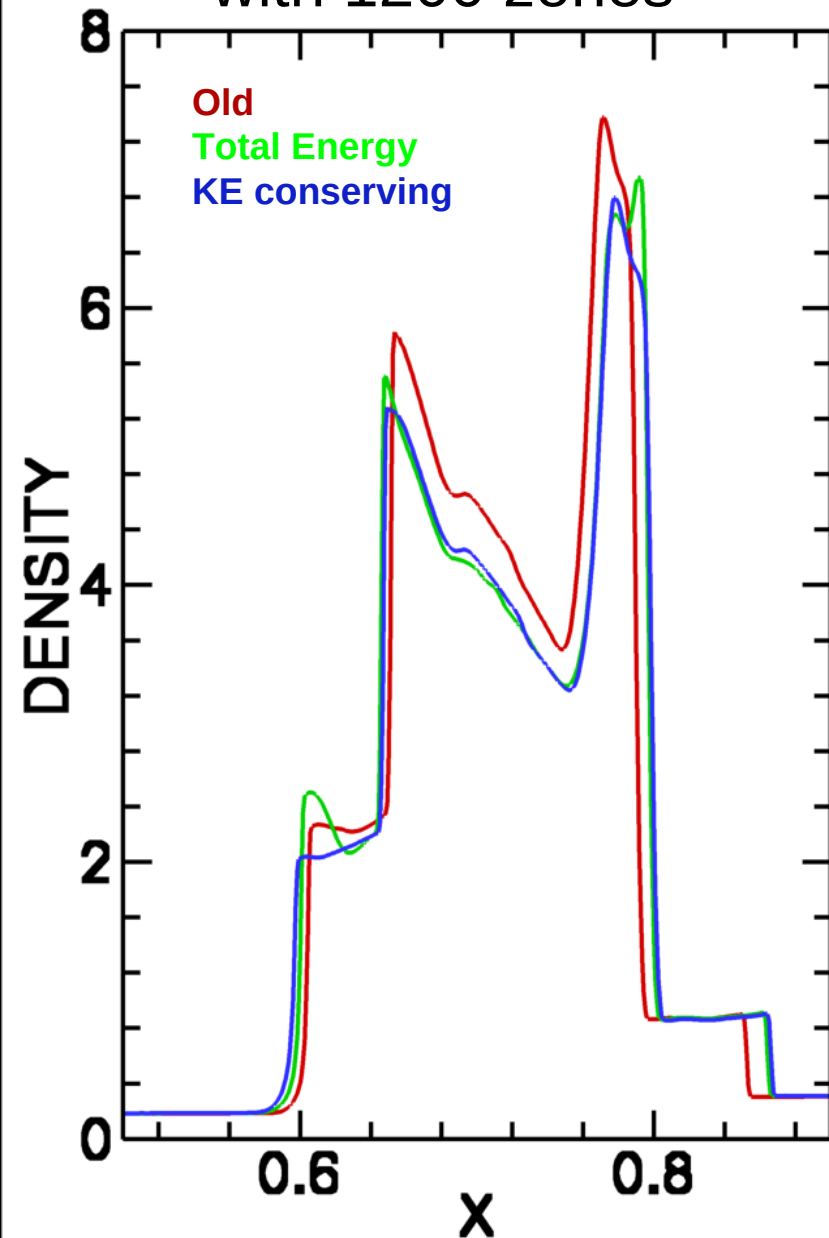


Results with Woodward-Colella (W-C) Blast Wave Problem

This demonstrates the ability of the KE conservation to produce correct results and is more flexible and robust



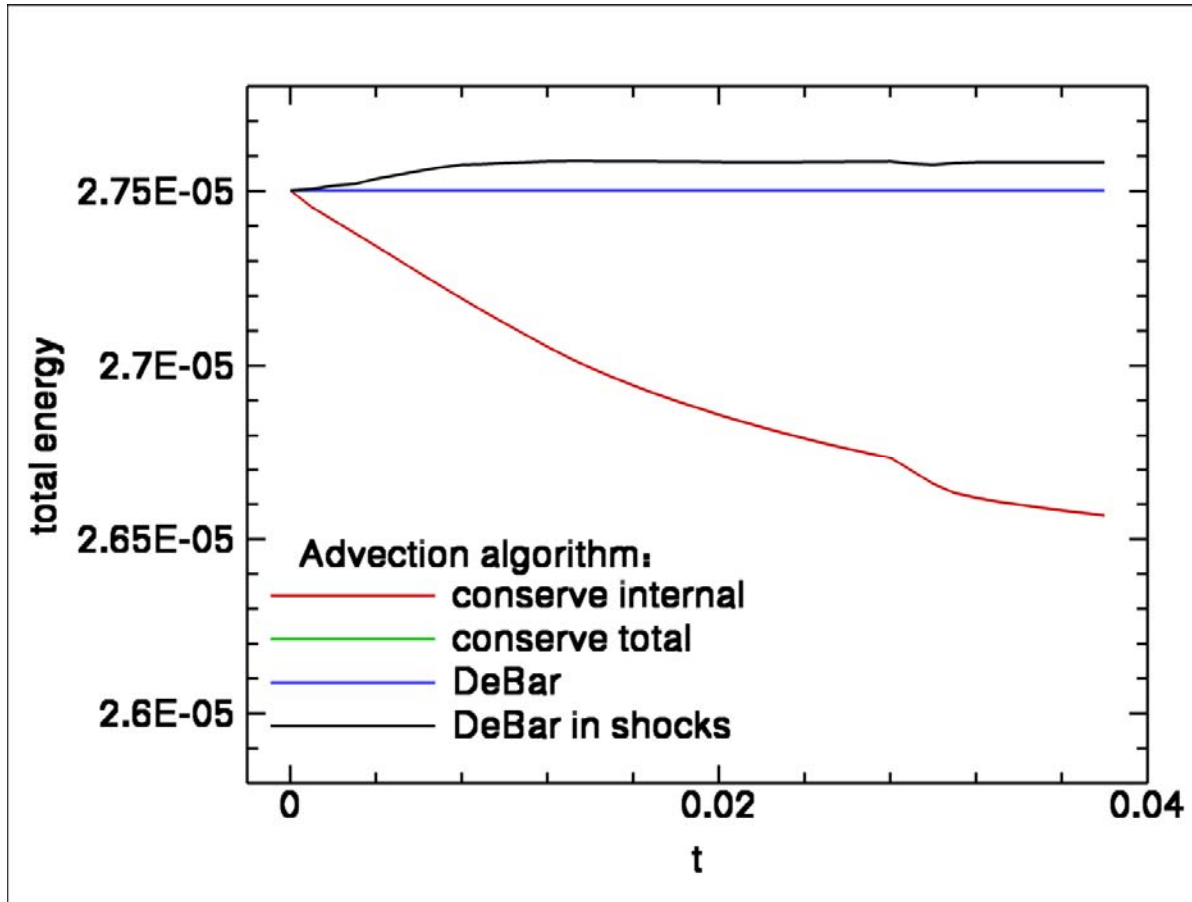
Alegra Results with 1200 zones





Results with W-C Blast Wave Problem (continued)

Total energy behavior - internal vs total energy advection vs DeBar & DeBar at shocks (with $Q/p > 0.001$)



The green curve is hidden by the blue curve.



Development of more physically realistic multimaterial treatment(s)

- Based on an isentropic relationship for multiple materials in a zone.
- The formal definition of bulk modulus can be viewed as the starting point, $B = -V \left. \frac{\partial P}{\partial V} \right|_s$
- From this relation and assuming that the flow is in pressure equilibrium, and changes are isentropic, we define $\sum_k f_k = 1$

$$\bar{B} = \left(\sum_k \frac{f_k}{B_k} \right)^{-1} \quad \bar{P} = \sum_k \bar{B} \frac{f_k}{B_k} P_k = \sum_k \beta_k P_k \quad \Delta V_k = \beta_k \Delta V$$



Pressure Relaxation

- Define the changes in the volume fractions, f_k to produce pressure equilibrium (and requisite energy changes),

$$\frac{\partial P_k}{\partial t} \approx \frac{P_k - \bar{P}}{\tau}$$

$$\frac{Df_k}{Dt} = f_k \frac{\bar{B} - B_k}{B_k} \nabla \cdot \mathbf{u} + \frac{f_k}{B_k} \frac{\partial P_k}{\partial t} \left(1 - \sum_k f_k \right) \approx \nabla \cdot \mathbf{u}$$

- Add in a pressure relaxation, and express the previous as an evolution equation,

$$\delta f_k = f_k \frac{\bar{B} - B_k}{B_k} \left(1 - \sum_k f_k \right) + \frac{f_k \Delta t (P_k - \bar{P})}{B_k \tau} \quad m_k \delta e_k = -\bar{P} \delta f_k$$

- + a void treatment (a whole talk by itself!)



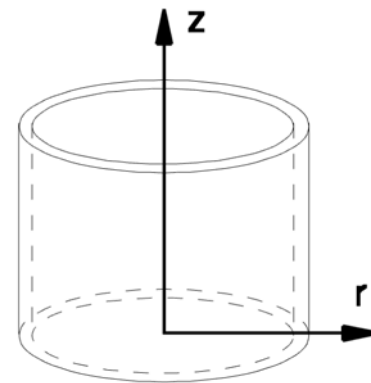
Prototype Z-pinch Problem

- Idea: Use $\mathbf{J} \times \mathbf{B}$ source term to help investigate hydrodynamics without invoking magnetics
- Enable code comparison
- Add acceleration to external forces (similar to gravity) and enables MMS expertise
- Developed by Jeff Banks and John Shadid
- Article in preparation
- Lumped-mass analysis with thin-shell approximation

A Magnetic Drive $\mathbf{J} \times \mathbf{B}$ Source Term for
Developing Prototype Z-pinch Shock-Hydro
Problems

$$\frac{d^2 R^*}{dt^{*2}} = - \left(\frac{I(t)}{I_{max}} \right)^2 \frac{1}{R^*}$$

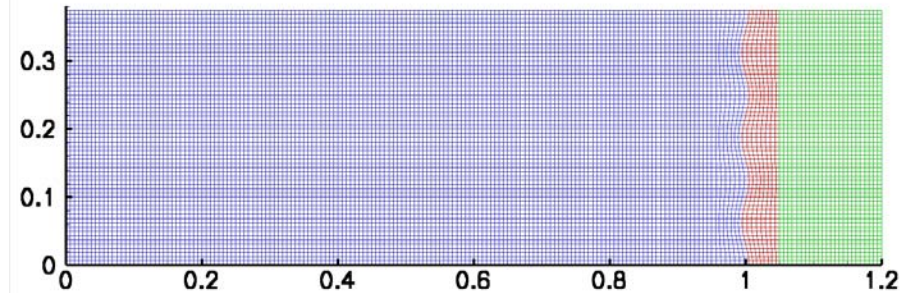
$$I(t) = \sqrt{12(1 - t^4)t^2}$$





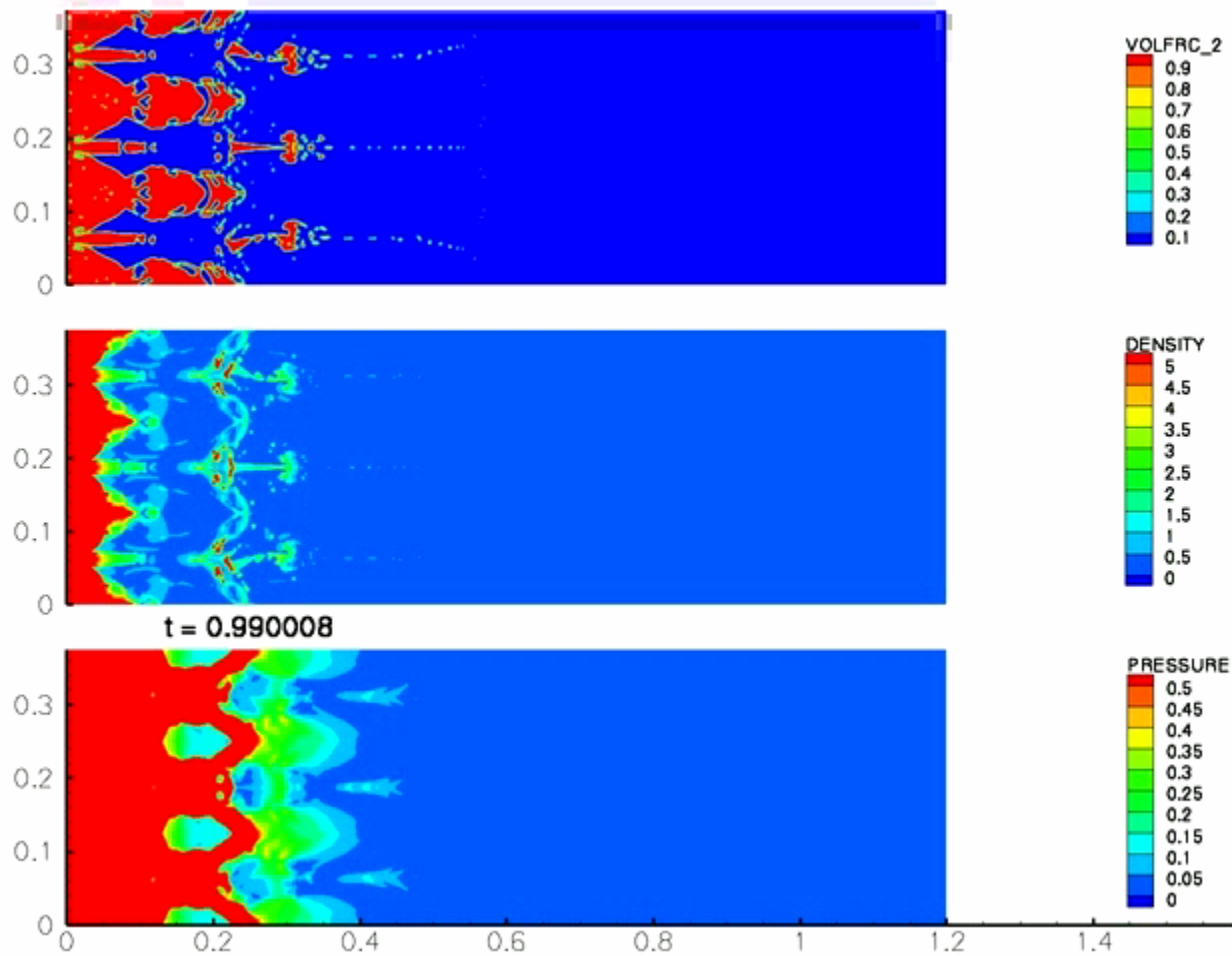
Multiple Materials

- Used 3 materials (all ideal gases)
 - Inside - $\rho = 0.05$, $T = 0.2$, $P = 0.01$
 - Liner - $\rho = 1.0$, $T = 0.01$, $P = 0.01$
 - Outside - $\rho = 0.025$, $T = 0.4$, $P = 0.01$
- Mesh
 - Course mesh: 192x60
 - Fine mesh: 768x240
 - Sinusoidal perturbation on inside of liner
- JxB source term applied only to liner material
- Used SMYRA Interface tracking
- **Problem exhibits**
 - Kevin-Helmholtz instabilities
 - Rayleigh-Taylor instabilities
 - Expansion oscillations (numerical)
 - Creates thin material “strings” -> good test of interface tracking



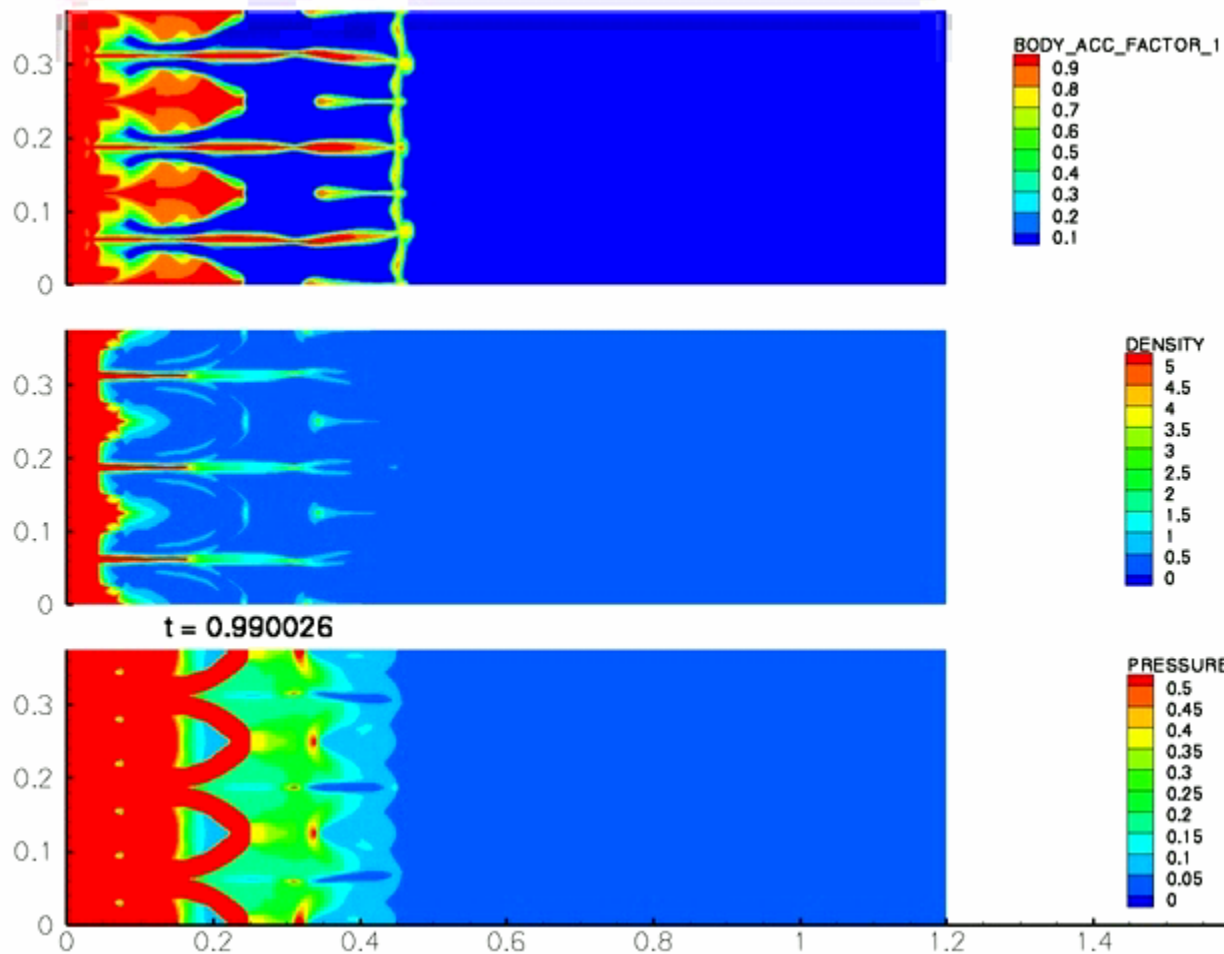


Multiple Materials





Single Material



- Needed to add tracer variable, λ , to mark JxB source term application
- Similar gross features



Modern Lagrangian scheme + limited artificial viscosity in progress

- The current Lagrangian method is nearly equivalent to the predictor step (conservative, but time-staggered) of a PC method.
- A corrector step for 2nd order is anticipated.
- In the process of developing a FEM compatible limited Q using a least square approach to computing a limiter.

$$Q = \rho \left(c_1 \bar{\Delta u} + c_2 (\bar{\Delta u})^2 \right); \bar{\Delta u} = \psi \Delta u$$

$$\psi = \sqrt{\frac{\sum (\Delta u - \nabla u \Delta x)^2}{\sum (\Delta u)^2}}$$

$$A^T A \bar{\nabla} = A^T \Delta u$$

$$\left\{ \begin{array}{l} A = \begin{pmatrix} \Delta x & \Delta y & \Delta z \\ \vdots & \vdots & \vdots \end{pmatrix} \quad \bar{\nabla} = \begin{pmatrix} \bar{\nabla}_u \\ \bar{\nabla}_v \\ \bar{\nabla}_w \end{pmatrix} \\ \Delta u = \begin{pmatrix} \Delta u & \Delta v & \Delta w \\ \vdots & \vdots & \vdots \end{pmatrix} \end{array} \right.$$

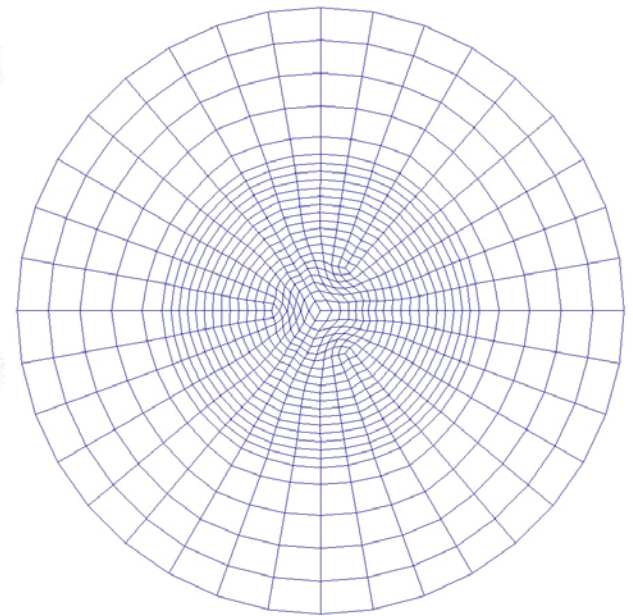
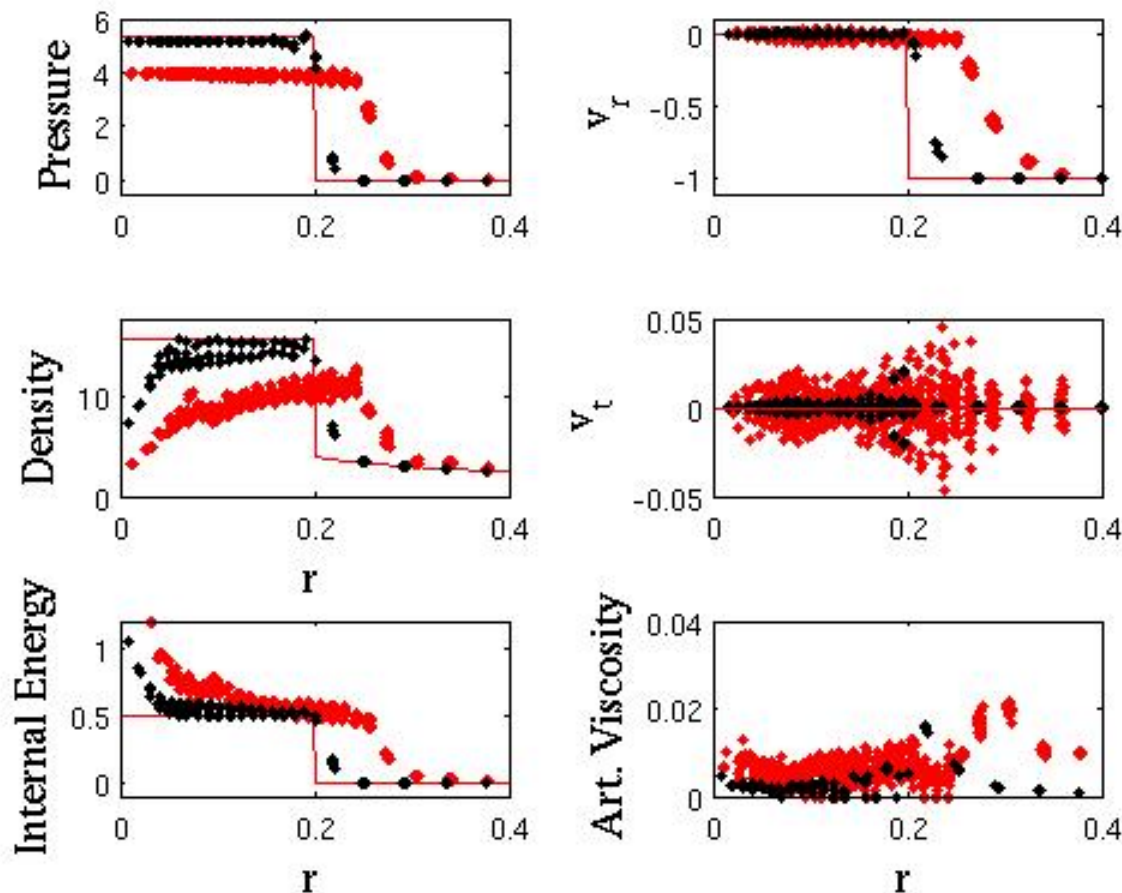


2nd order P-C with a limited Q results: Noh's problem-very coarse mesh

Black = New Q

Red = Old pronto Q

Trisection Mesh
w/new Q
(Research code)

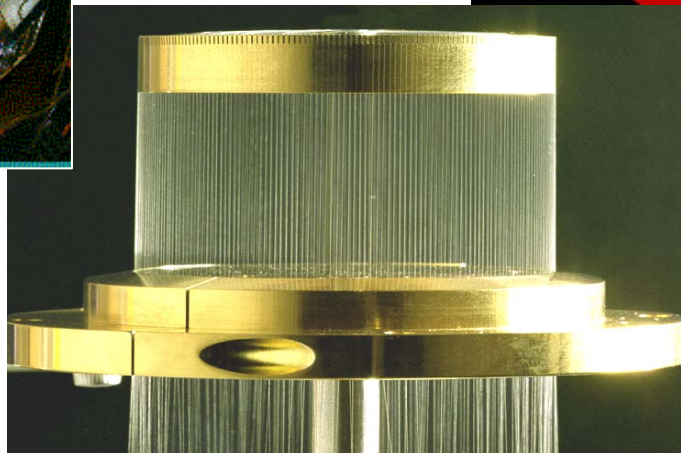
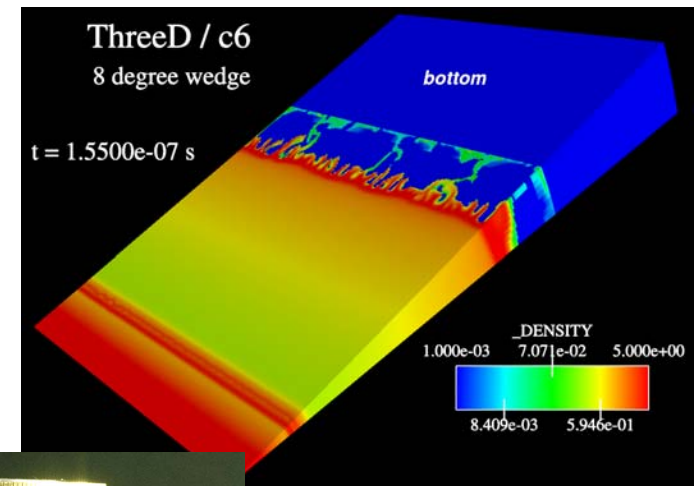




Demonstration of Algorithm

Impact: Z-Pinch Implosion

- A simulation of a wire array implosion on the Z-machine at SNL





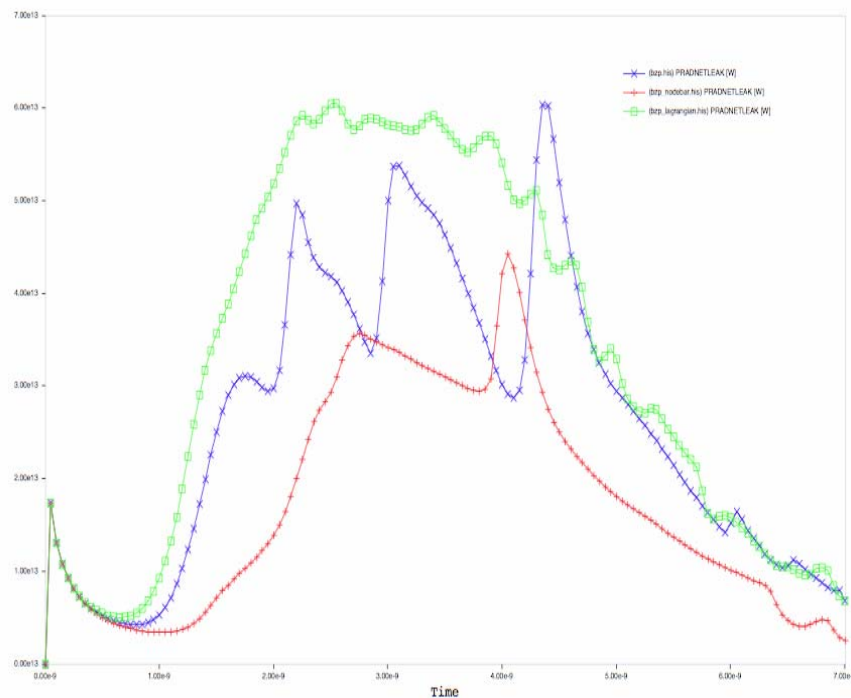
Results with Simplified Z-pinch

- Results of radiation output from a 1-D implosion (comparing Lagrangian w/Eulerian)

Lagrange

Eulerian DeBar

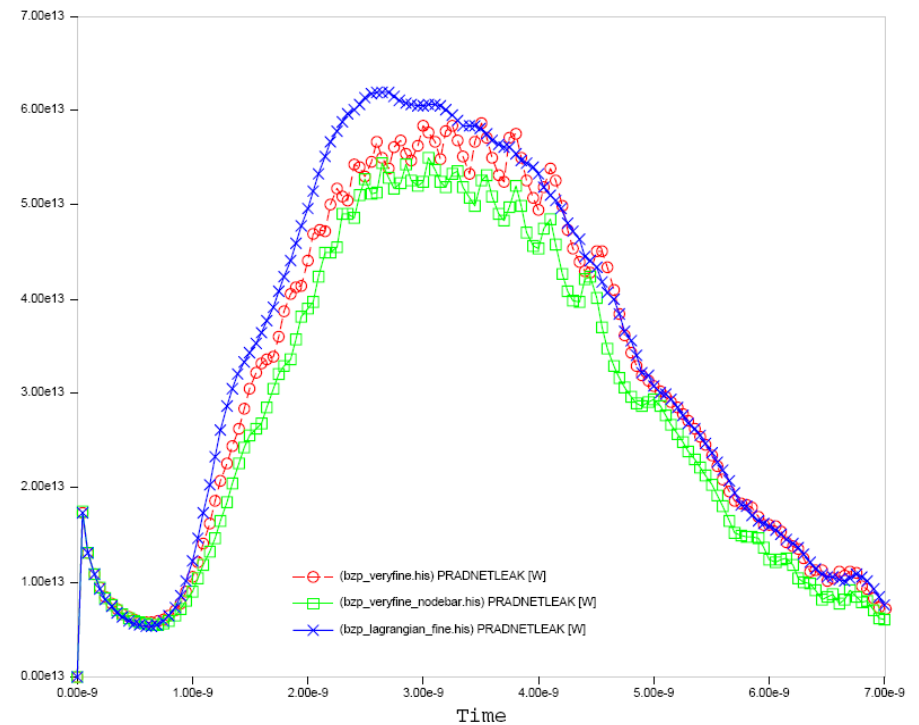
Eulerian No DeBar



Lagrange (4x)

Eulerian DeBar (4x)

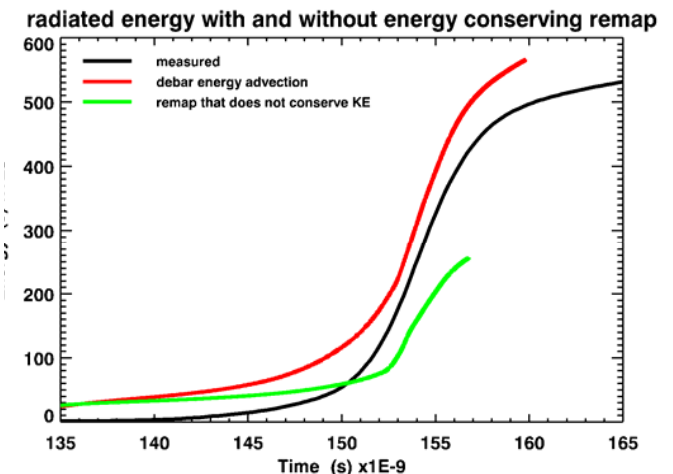
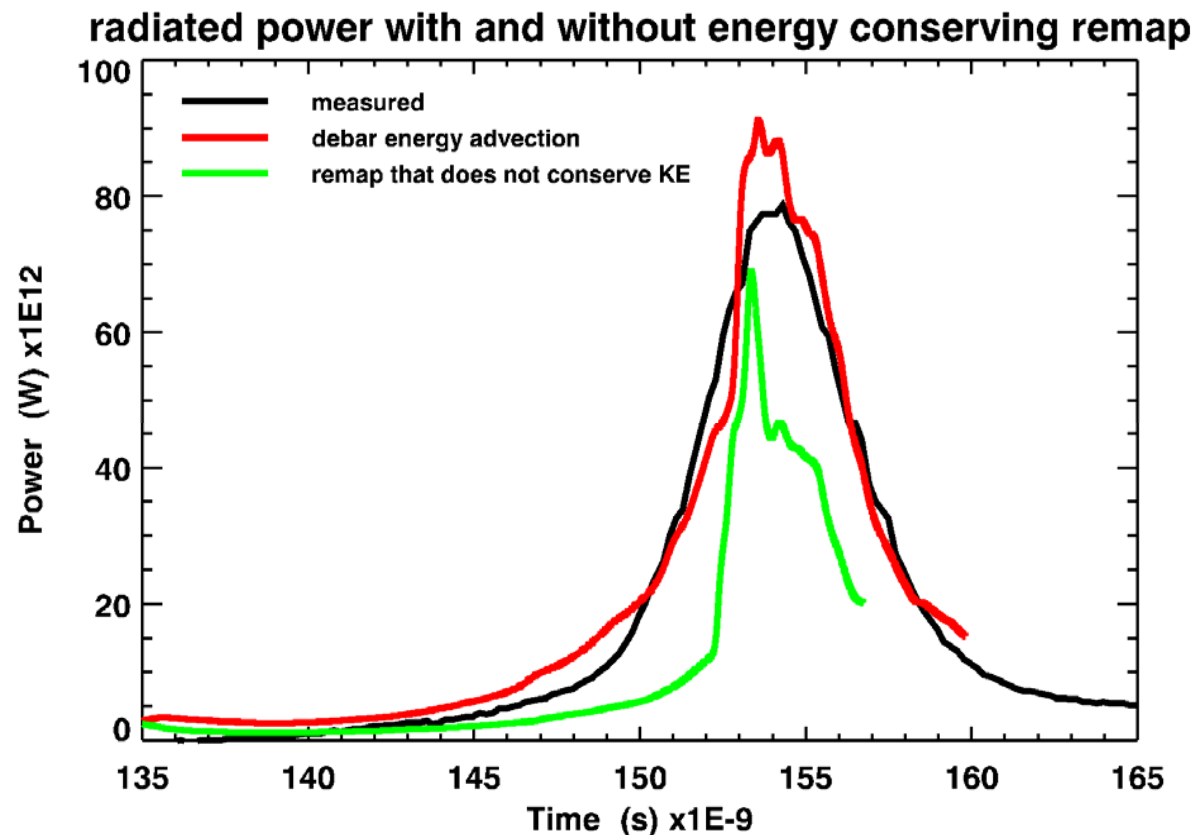
Eulerian No DeBar (4x)





Demonstration of Algorithm Impact: Full 3D Z-Pinch Implosion

- This shows the impact of conserving energy. The radiated power is the key metric.





Summary

- **Alegra has benefited from the focus on several problem areas.**
- **In association with an emphasis on testing, Alegra's algorithms have been improved and tests are being placed in a permanent repository.**
- **These improvements have provided tangible benefits for Alegra's HEDP applications.**



Future Directions

- **The algorithms need to continue improvement in both remap and Lagrangian hydro.**
- **A more modern Lagrangian hydro method is needed (modern Q + bonafide 2nd order in time predictor-corrector).**
- **The testing process needs to expand in both breadth, depth and ease of use to support a sustained V&V evidence base.**