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Void's Unphysical Response In Hydrocodes

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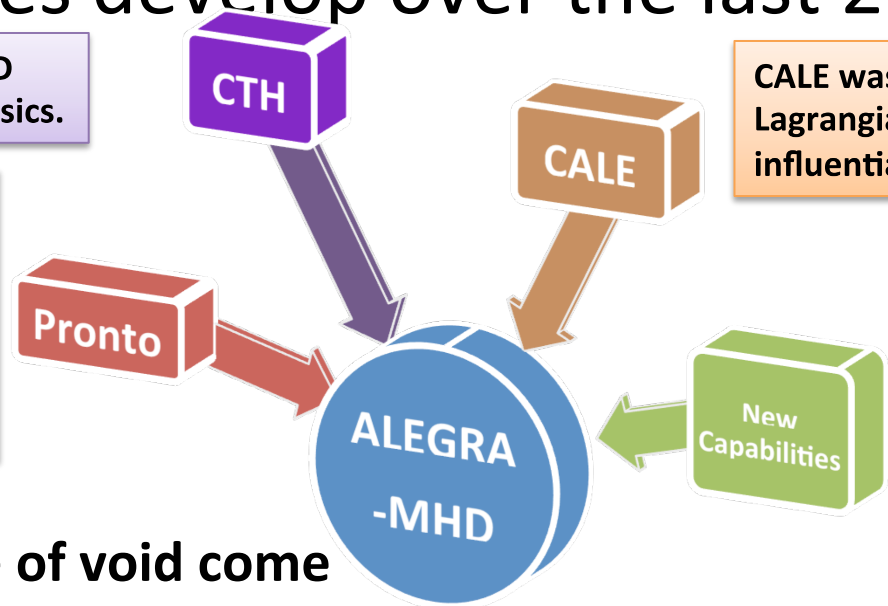
“A vacuum is a hell of a lot better than some of the stuff that nature replaces it with.”–Tennessee Williams

ALEGRA is a hydrocode with specific multi-physics capabilities develop over the last 20+ years.

CTH is a fixture in the DoD community for shock physics.

CALE was an early arbitrary Lagrangian-Eulerian (ALE) code influential for ASC.

SNL code capabilities: Pronto was a mid-1980 Lagrangian solid dynamics code and is a predecessor to SIERRA-MECHANICS today (Presto).



LDRD has contributed to the large scale linear algebra (TRILINOS), material modeling (QMD/DFT-MD), XFEM and railgun/coilgun simulation capability.

Where does our use of void come from? CTH

- **Void is used in CTH in several capacities.**
- **It is introduced to make fracture and spall volume filling.**
- **If material is discarded, it is replaced with void (cell doctor)**

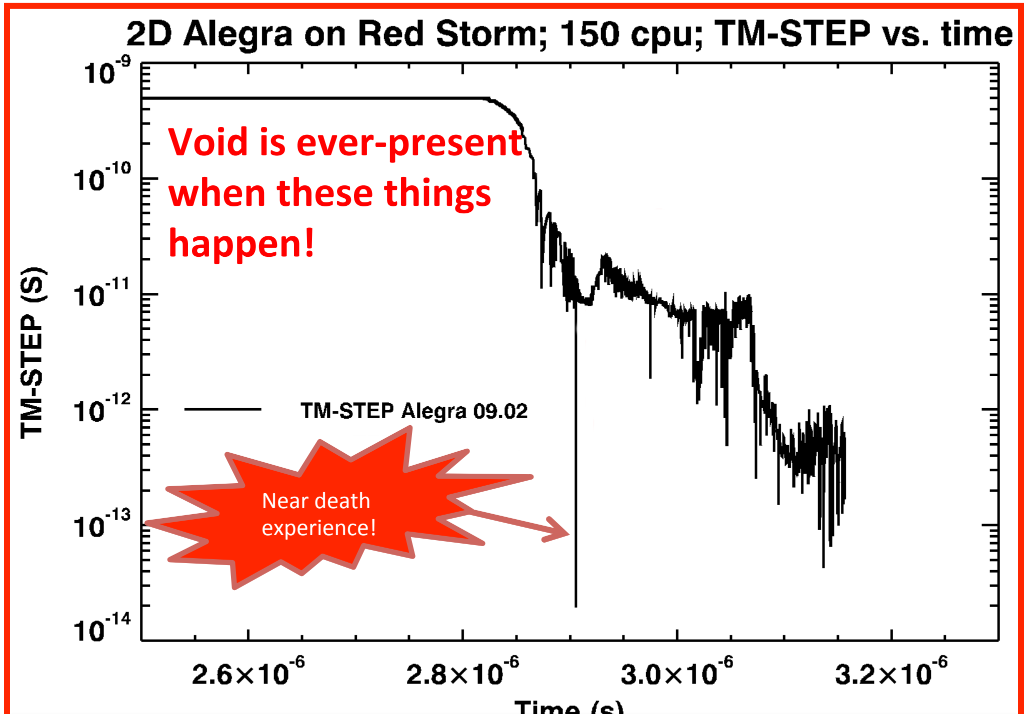
What key defining capabilities does ALEGRA possess?

- Mimetic magneto-hydrodynamics (MHD), circuit modeling
- Extended finite element (XFEM) under development
- High fidelity material modeling (especially for MHD)
- Ceramic material models
- Optimization and UQ linkage to DAKOTA
- Robust modeling of high-strain rate deformation.

Six years ago: With growing use on more complex problems, significant issues arose due to code robustness.

- Users **wanted calculations to be reliable.**
- **Our continued support depended upon improving reliability and resilience.**
- **Many important calculations did not complete due to a variety of issues.**

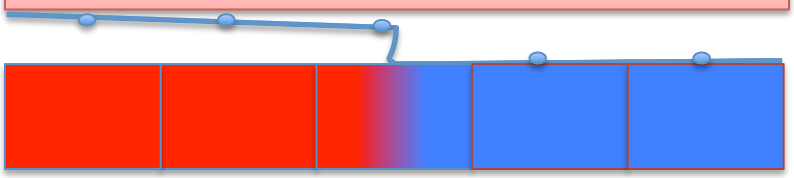
- **Users had grown to expect the code to not reliably work for very challenging problems.**
  - **They expected the code to fail!**
  - **Some users wouldn't even report problems because it was the norm.**



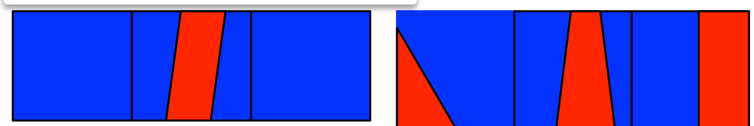
This plot shows a typical time step trace for ALEGRA in this time period. The time step "dropouts" were common as was the general decay in the magnitude of the time step. Calculations either failed or became untenable due to small time step size.

We made improvements in the remap and multimaterial methods plus the stability criteria.

Summary of remap changes: Detect the local multimaterial flow topology



Problem configurations



Third-order remap based on three element parabolic conservative interpolation.

- **For robustness, the edge values are third-order, but bounded by neighbors,**

$$\phi_{j+1/2} = \tfrac{1}{6}\left(2\phi_{j+1} + 5\phi_j - \phi_{j-1}\right) \rightarrow \tfrac{1}{2}\left(\phi_{j+1} + \phi_j\right) - \tfrac{1}{6}\left(\Delta_{j+1/2}\,\phi - \Delta_{j-1/2}\,\phi\right)$$

$$\Delta_{j-1/2}\,\phi = \min\mathrm{mod}\left\lfloor \phi_j - \phi_{j-1}, 4\left(\phi_{j+1} - \phi_j\right)\right\rfloor$$

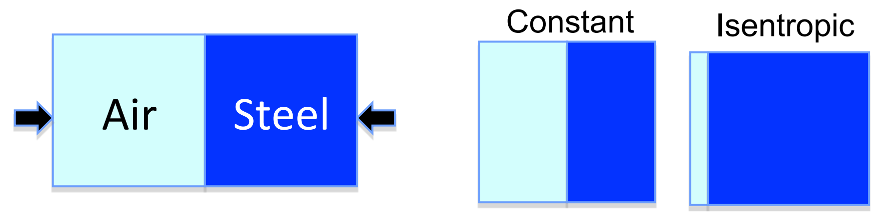
Mixed cell remap is now lower order

- **ALEGRA uses the minmod scheme (the most dissipative second order "TVD" method)**

$$\phi_{j+1/2} = \phi_j + \tfrac{1}{2}\min\mathrm{mod}\left\lfloor \phi_{j+1} - \phi_j, \phi_j - \phi_{j-1}\right\rfloor$$

- **Effectively uses one-sided differencing in mixed cells, only differencing into the pure material region (closer values).**

Summary of multimaterial Lagrangian closure algorithm changes provide a physically based stable model (void is a "thorn in the side" of this algorithm)



constant volume $\quad \dfrac{df_k}{dt} = 0$

$$\frac{df_k}{dt} = f_k\left(\frac{\overline{B} - B_k}{B_k}\right)\nabla\cdot u - \frac{f_k}{\overline{p}}\frac{dp_k}{dt}$$

Summary of time step size calculations: based upon the Fourier analysis of the Lagrangian step with dissipation.

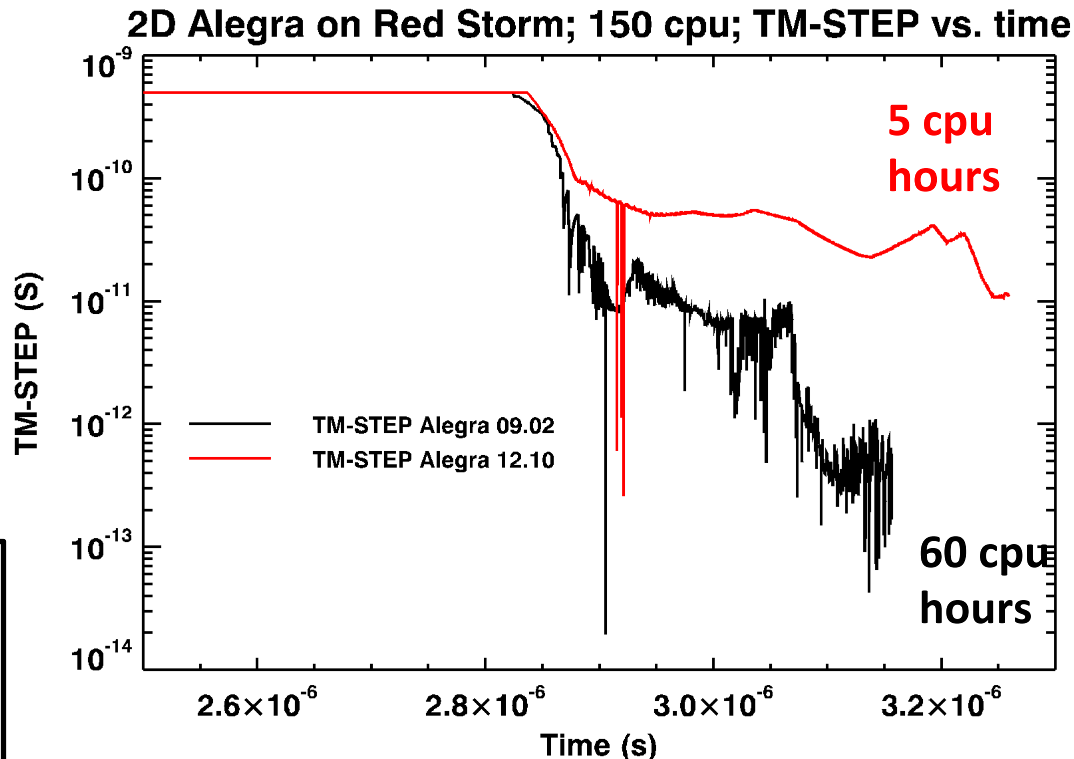
$$\Delta t_2 = \frac{h}{c\left(\sqrt{1+\eta_{\max}^2} + \eta_{\max}\right)} \qquad \eta_{\max} = c_1 + c^{-1}c_2 h\left|\nabla\cdot v\right|$$

Our existing user base stood up and took notice of the changes we made.

- The HEDP continued to rely upon ALEGRA for experimental design despite lack of direct support.
- In December 2008, I received the following e-mail from the lead designer (Ray Lemke, 1641) for EM flyer experiments:

Excerpted From Ray Lemke, Dec 11, 2008 e-mail:

…I though you would be interested in this timing result. A large 2D Alegra MHD/thermal-conduction simulation (**655,000 elements**) I've been running on **150 nodes of Red Storm** completes **more than 10 time faster …** (~5 hrs completion time vs. ~60 hrs, respectively)…



ALEGRA was 12 times faster than before!

There are big problems with void

Lunch with Misha

- Allen and I had lunch with Misha at Multimat last year
- He is interested in exploring how everyone does void (and everyone is doing it in an ad hoc manner)
- Misha outlined several test problems we should run:
  - Void closure, 1 and 2-D
  - Free expansions, and shock through material and into void (JOWOG, NECDC possibilities)

Misha Shashkov proposed a set of problems to us at Multimat 2013 in San Francisco

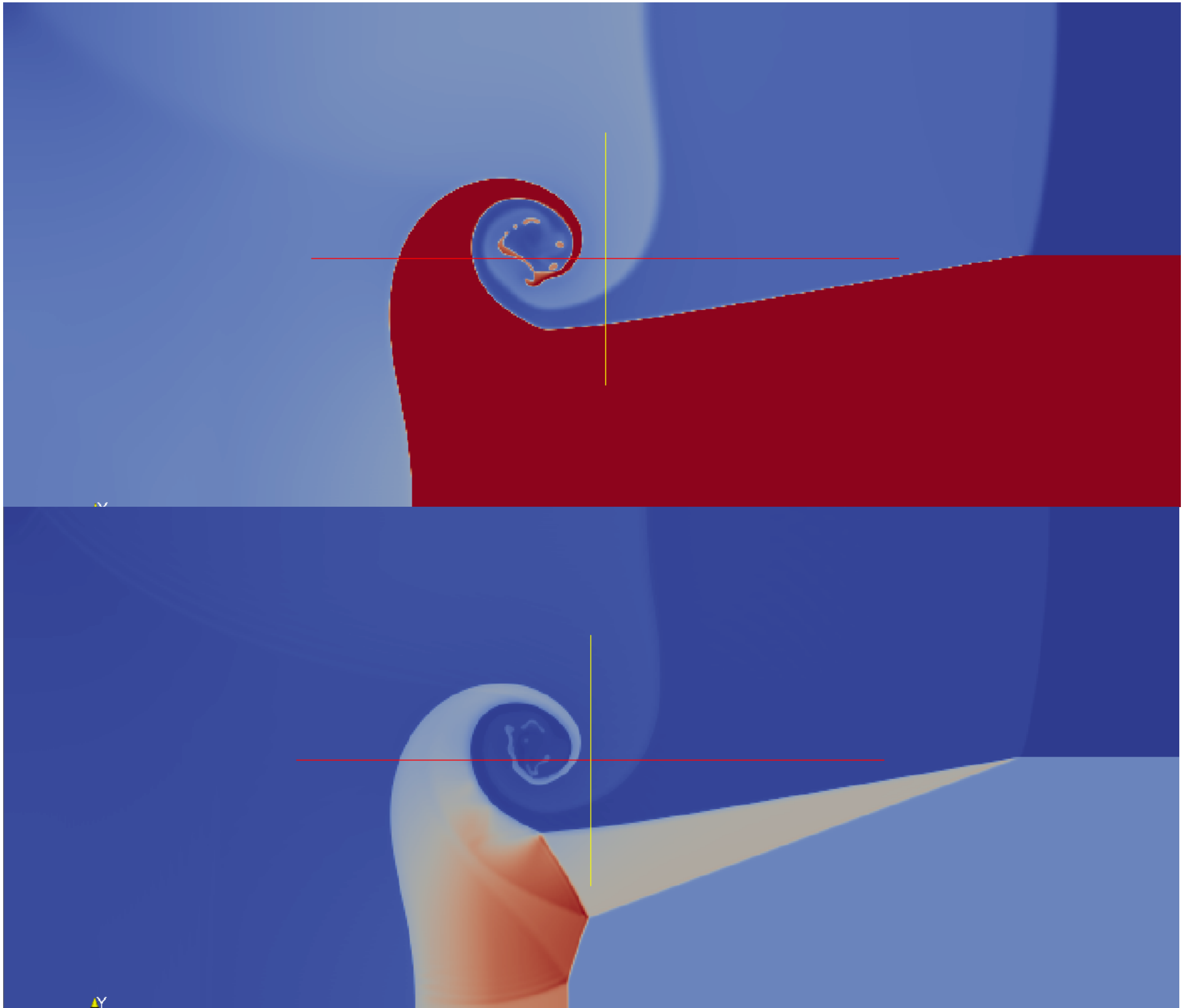
- He set four problems:
  - Free expansion
  - Blast wave propagating into void
  - Void closure in 1-D
  - Void closure in 2-D
- We have started to set up and solve these with ALEGRA.
- We know the free expansion problem is an issue… it does not converge to the right answer
- We strongly suspect other codes have similar issues and we can interact on this topic.

"I'm gonna make him an offer he can't refuse"
– The Godfather

New Test Problems

- Triple Point Series
  - Single material
  - Multimaterial
  - Asymptotically strong
- Void problems
  - Void Closure (material closes out void, results are good)
  - Void Expansion (no version of ALEGRA solves correctly, other codes share this problem)
  - Blast to void

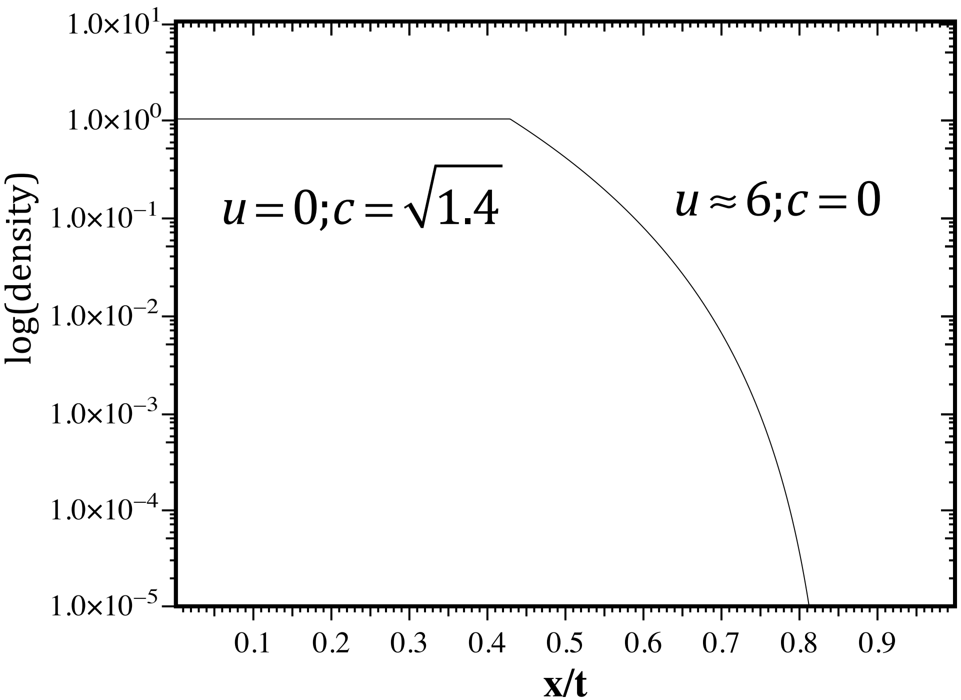
Triple Point Results are reasonable

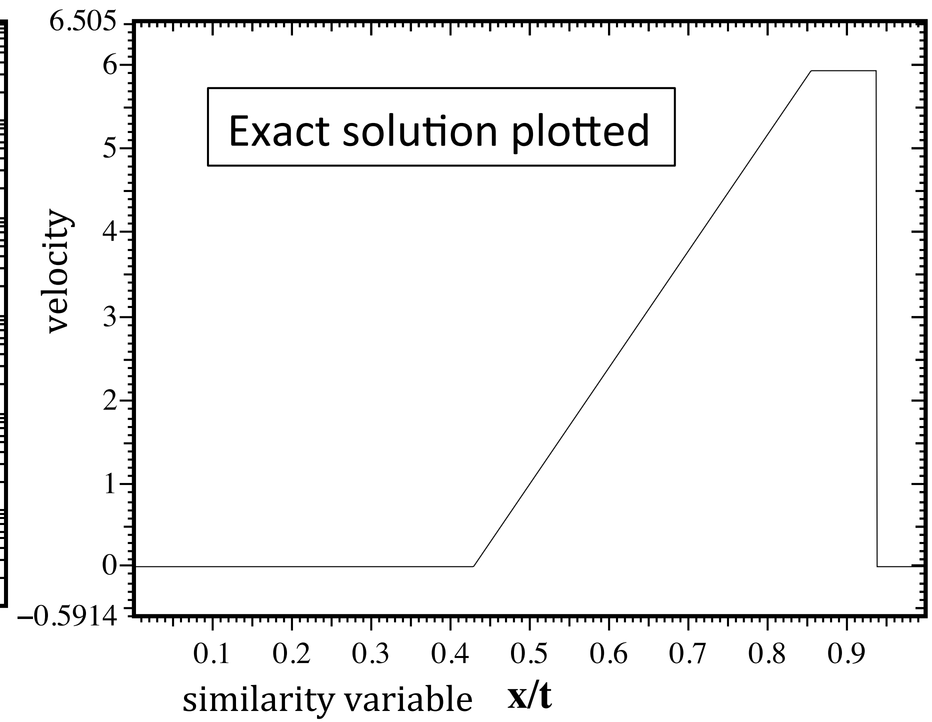


"Just because there's an exact formula doesn't mean it's necessarily a good idea to use it."- Nick Trefethen

Void expansion results have asked more fundamental questions of the code

- Stability issues associated with the expansion problem highlight a fundamental oversight

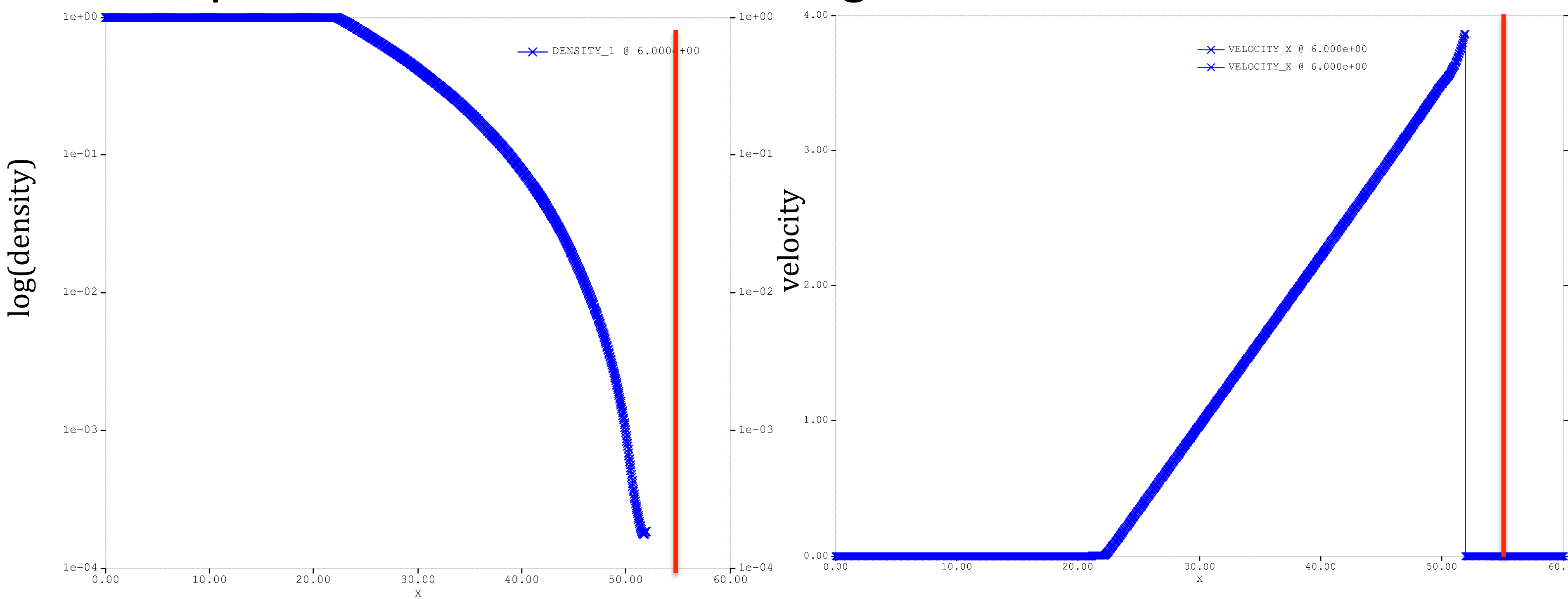




The characteristic speed at the free surface is 5 times larger than the initial conditions arising from a change in pressure (Δp)

ALEGRA solutions do not converge to the analytical solution

- Nothing else does either as far as we know…
- The solution is fundamentally flawed, no set of options helps. The solution will never get to the exact one.

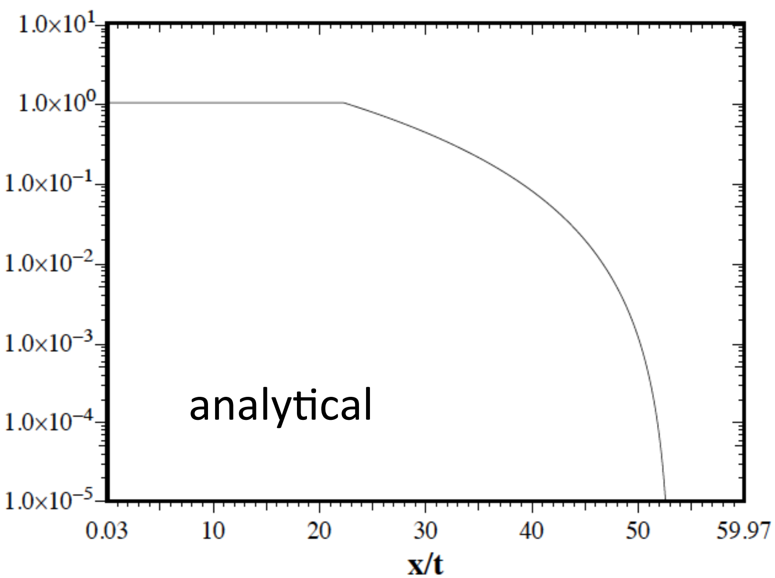


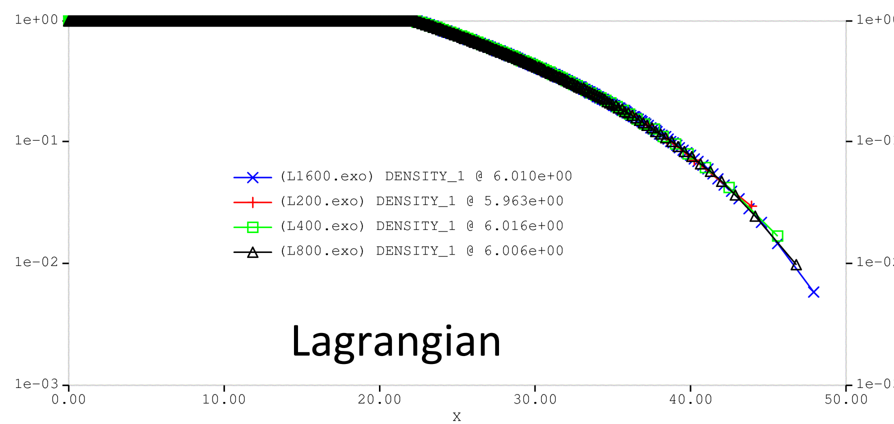
- XFEM is actually worse. Something really bad is happening, and we don't know what it is.

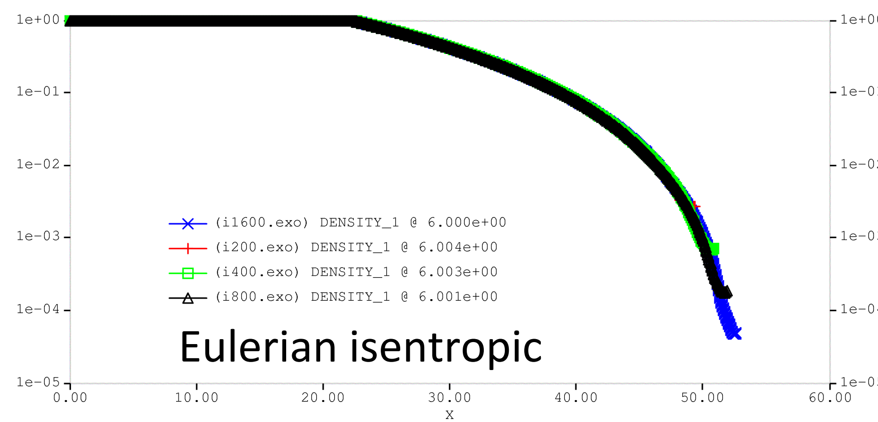
The free expansion problem

- We have an exact solution via the asymptotic limit of a Riemann solution
- The velocity of the free surface is analytical,

$$V_{F.S.} = V^0 + \frac{2a^0}{\gamma - 1}$$







Convergence of the free expansion

- We look at the problem on several meshes at t=6.0, $V_{F.S.}$=3.87. $X_{F.S.}$=53.24
- Default (isentropic MM)

$$54.24 - 8.78\Delta x^{0.51}$$

- Lagrangian

$$51.75 - 8.69\Delta x^{0.42}$$

- Default (CV MM)

$$54.88 - 8.71\Delta x^{0.45}$$

- XFEM

1st order remap

$$54.65 - 12.53\Delta x^{0.37}$$

2nd order remap

$$54.59 - 11.13\Delta x^{0.48}$$

Almost identical issues show up with a cell-centered Eulerian calculation

- When the expansion into vacuum problem is run with an Eulerian cell-centered code using Riemann solvers, and Piecewise linear or parabolic reconstruction, the problems persist.
- No convergence
- Stability problems
- This isn't just a Lagrangian or ALE or staggered mesh issue.

The Expansion into void may induce numerical instabilities

- The standard time step estimate may be inadequate because the expansion into void induces dynamics that are faster than the stability estimate.
- Analysis is ongoing to produce a practical solution to this problem.
- The basic idea is to use existing velocity and pressure differences to estimate changes in the characteristic speeds.
- These estimates can then be used to produce a stable time step size estimate.
- This is straightforward for ideal gases, but harder for real materials. We don't want to get an overly conservative time step estimate either.

“Von Neumann told Shannon to call his measure entropy, since ‘no one knows what entropy is, so in a debate you will always have the advantage.’ ”

— Jeremy Campbell

Stability and dissipation are intimately related to each other

- Theory of hyperbolic conservation laws

$$\frac{\partial U}{\partial t}+\frac{\partial F(U)}{\partial x}=0 \rightarrow \frac{\partial U}{\partial t}+\frac{\partial F(U)}{\partial U}\frac{\partial U}{\partial x}=0 \rightarrow \frac{\partial U}{\partial t}+A\frac{\partial U}{\partial x}=0$$

- This linearization can be analyzed to give the eigenvalues. These eigenvalues are used to define the stability limit.

$$A=R\lambda L;\lambda=\left(-c,0,c\right)$$

- We could get the full stability limit through solving the Riemann problem exactly
  - what was used to create the plots on the previous slide, this takes about 16 iterations of Newton's method in that case! Always converging from below

A second order expansion of the analysis offers an answer to the issue

- Take the nonlinear flux and expand it,

$$F(U)=F(U_0)+\frac{\partial F(U_0)}{\partial U}\delta+\frac{1}{2}\frac{\partial^2 F(U_0)}{\partial U^2}\delta^2+O(\delta^3)$$

- Plug this back into the PDE we started with

$$\frac{\partial U}{\partial t}+\frac{\partial F(U)}{\partial x}=\frac{\partial (U_0+\delta)}{\partial t}+\frac{\partial F(U_0)}{\partial x}+\frac{\partial F(U_0)}{\partial U}\frac{\partial \delta}{\partial x}+\frac{1}{2}\frac{\partial^2 F(U_0)}{\partial U^2}\frac{\partial \delta^2}{\partial x}+O(\delta^3)$$

- Analyze – usually on the first term is carried,

$$\frac{\partial F(U_0)}{\partial U}=R_k\lambda_k L_k;\frac{\partial^2 F(U_0)}{\partial U^2}=\frac{1}{2}(\lambda_j-\lambda_k)L_i\overset{\boxed{\approx 0}}{\left(R_k\cdot\nabla_U R_j-R_j\cdot\nabla_U R_k\right)}+\delta_{ik}\left(R_j\cdot\nabla_U\lambda_i\right)$$

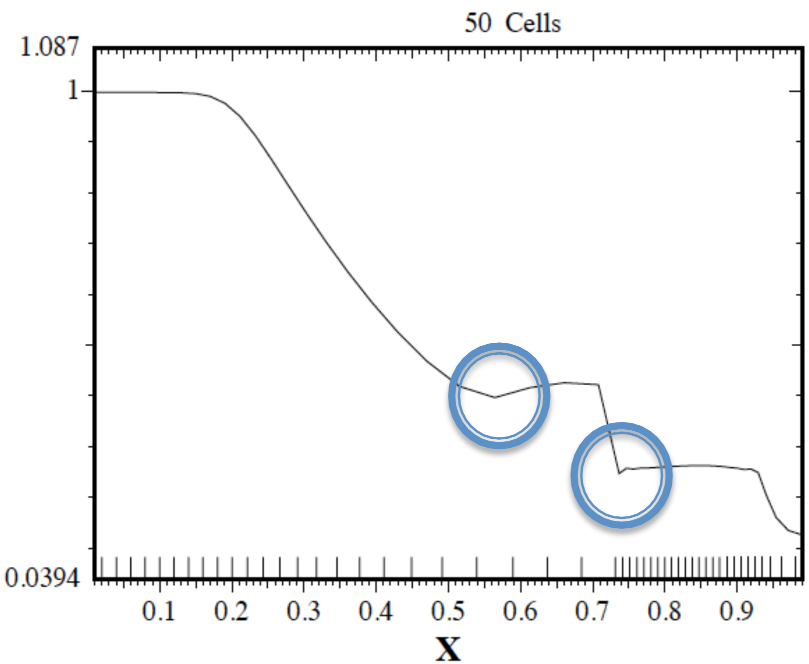
- We expand the second order term (see e.g., Lax, Dafermos, and Roe & Balsara)

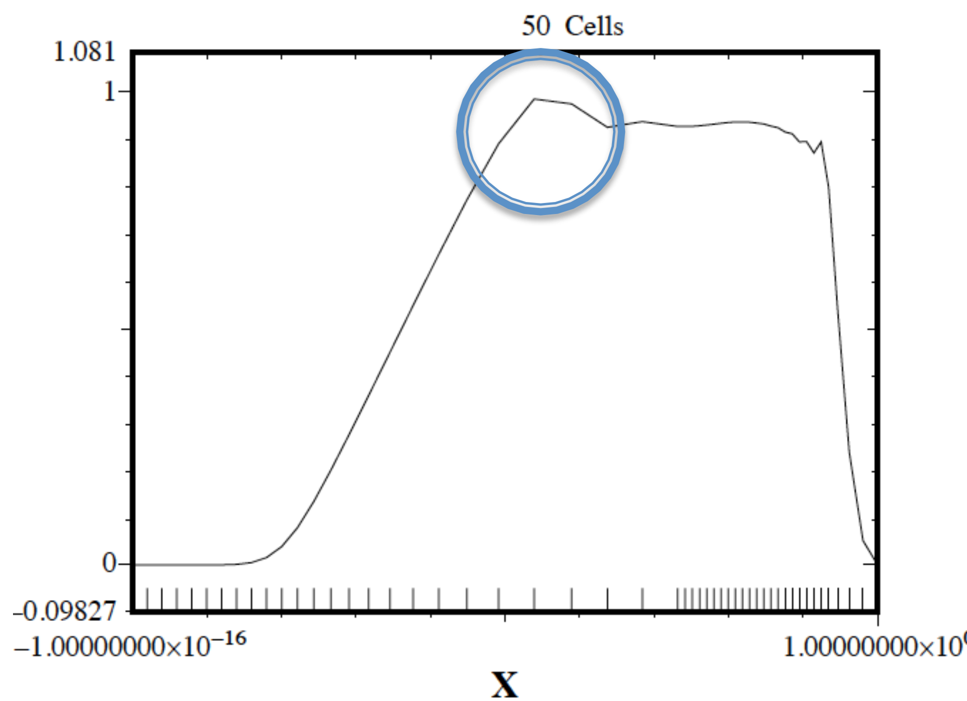
$$\lambda_k(U)=\lambda_k(U_0)+\left(R_k(U_0)\cdot\nabla_U\lambda_k(U_0)\right)L_k(U_0)\partial_x U$$

Diagnosis:
Is this an entropy violating solution?

Lax Entropy Condition – Valid Shock $$\lambda_L > \lambda > \lambda_R$$

Lax Entropy Condition – Valid Expansion $$\lambda_L < \lambda < \lambda_R$$





Connection to artificial viscosity

- Usually the first order term defines the stability of the integration, i.e.,

$$\Delta t \le \frac{\Delta x}{|u| + c} \text{ or } \Delta t \le \min\left(\frac{\Delta x}{|u|}, \frac{\Delta x}{c}\right)$$

- We are proposing including the second order term, (for u & p, Δ's in space)

$$\Delta t \le \frac{\Delta x}{|u| + c + \frac{\gamma+1}{4}\left(|\Delta u| + \frac{|\Delta p|}{\rho c}\right)} \text{ or } \Delta t \le \min\left(\frac{\Delta x}{|u|}, \frac{\Delta x}{c + \frac{\gamma+1}{4}\left(|\Delta u| + \frac{|\Delta p|}{\rho c}\right)}\right)$$

- These same ideas are used to define the level of numerical dissipation, usually the first term is used, but the second term also defines the quadratic part of the Q.

$$Q = c\,\Delta u + \frac{\gamma+1}{4}\left(|\Delta u| + \frac{|\Delta p|}{\rho c}\right)\Delta u$$

For dissipation via artificial viscosity, Riemann solvers and time step estimates

- We might do well to work with estimates of wave speeds that are bounding the “truth” from above, not below
- Riemann solver iterations might start with estimates that are larger than the solution
- The same for time step sizes.

“Nature abhors a vacuum.”
–Francois Rabelais

Recent progress has focused on the nature of the velocity at nodes

- The nodal "velocity" is really a conserved quantity, the momentum of the node
- We can recover the velocity at the nodal point and use this to move the nodes

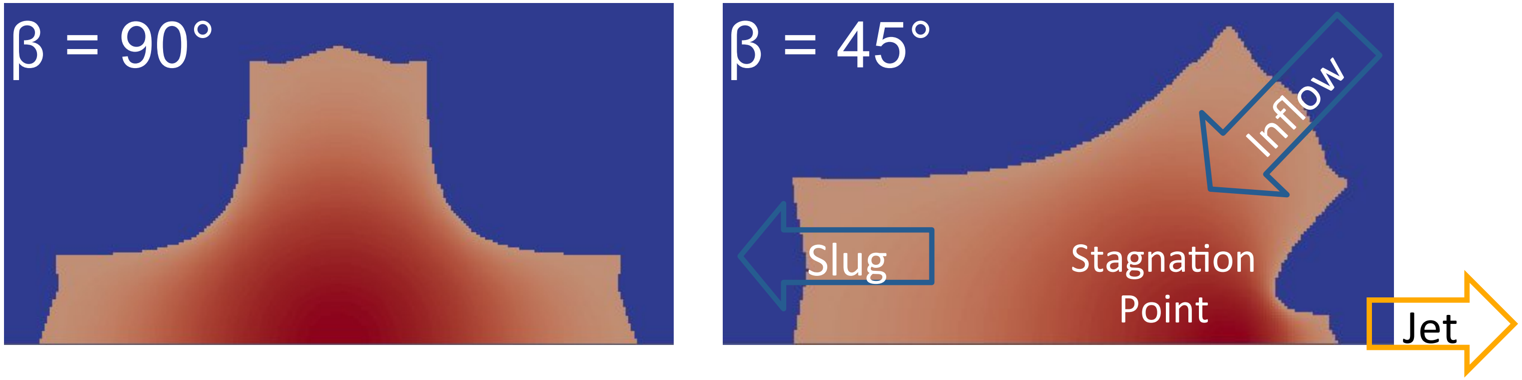
$$u = \langle u \rangle - \frac{h^2}{24}\Delta^2 u$$

- This improves the solution notably and lessens the entropy violations.
- It does not fix things, it makes them better.
- Should this velocity be used for the energy?

“We become aware of the void as we fill it.” — Antonio Porchia

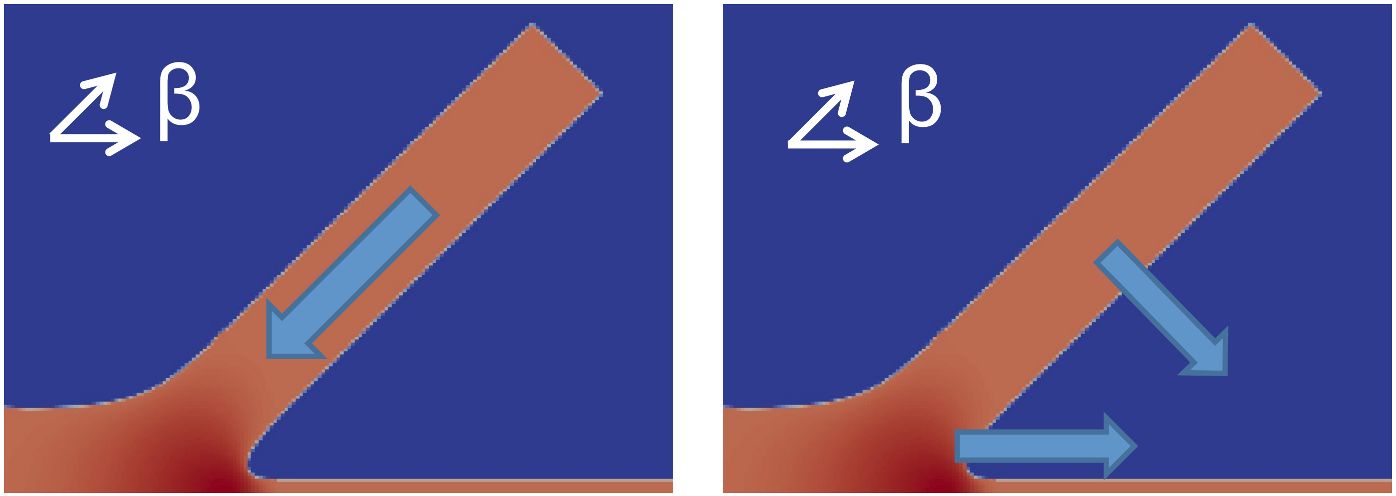
We are using a complex test problem with an exact solution to run our code through the "ringer"

CJETB code exodus solutions



Simulations – 2 incident angles, 2 frames of reference

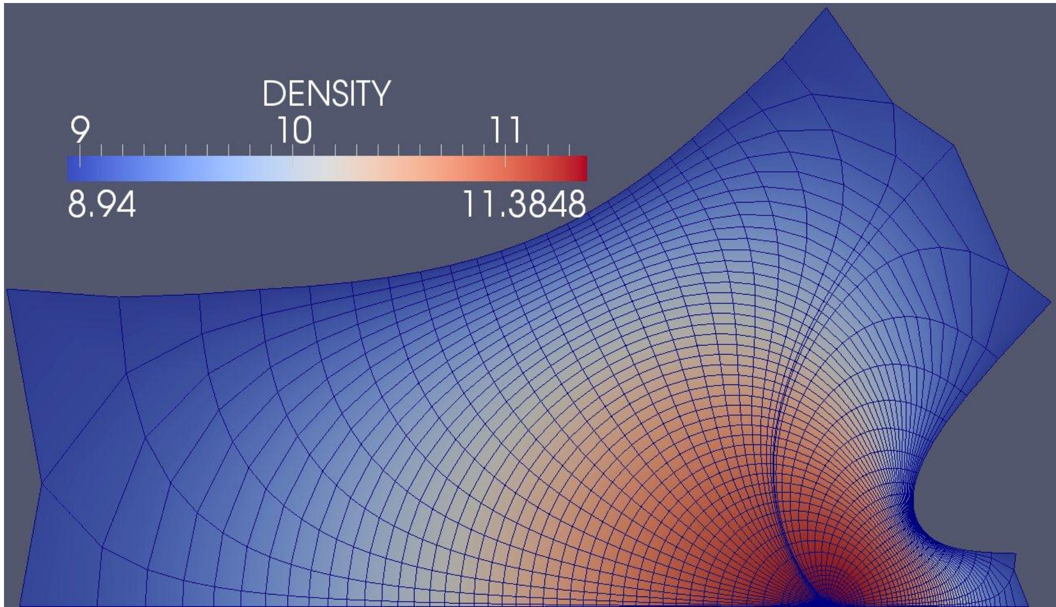
Stagnation Point Frame of Reference



Laboratory Frame of Reference

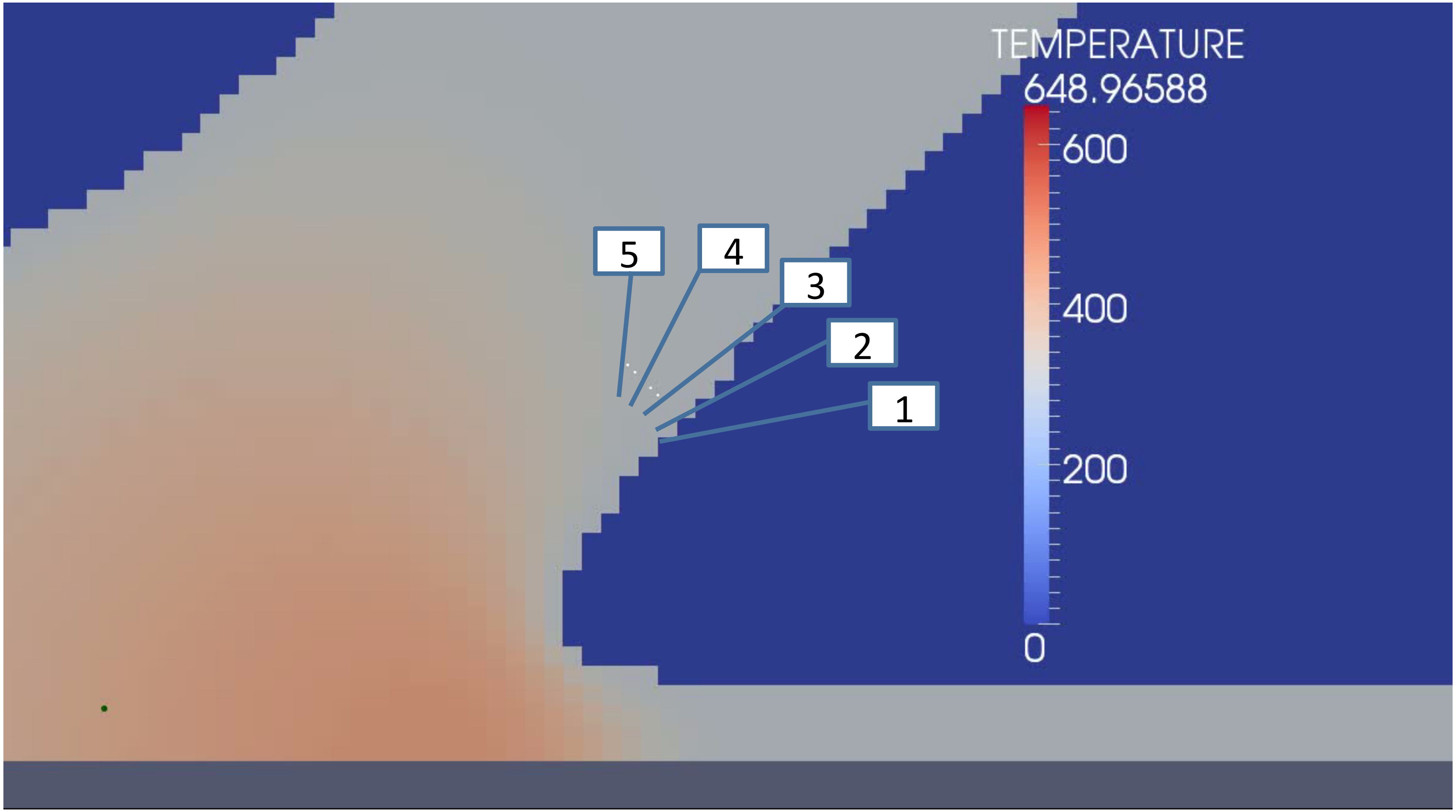
Exact Solution

- Complex difficult problem with simple characteristics
- – Steady Plane Subsonic Isentropic Fluid Flow (no strength)
- – Complex analytical representation (cjetb.f code) provides a solution on an exodus mesh. Robinson SAND2002-1015.
- – Solution imported to ALEGRA using diatoms exodus solution import
- – MG Murnaghan EOS Model
  - Two free reference curve parameters, valid for low compression
  - Simplified version of MG US UP useful for V&V



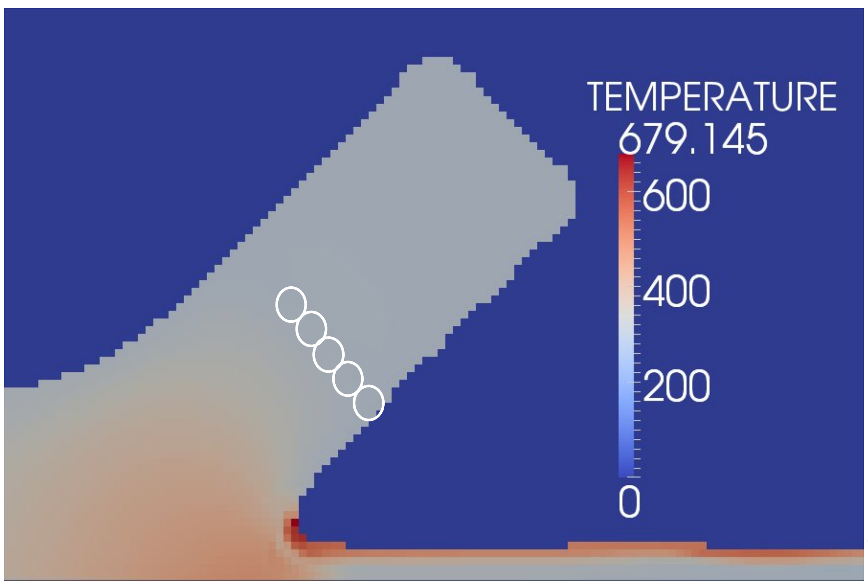
Lagrangian Tracers

In future slides, numbered tracers refer to the distance from the edge of the jet

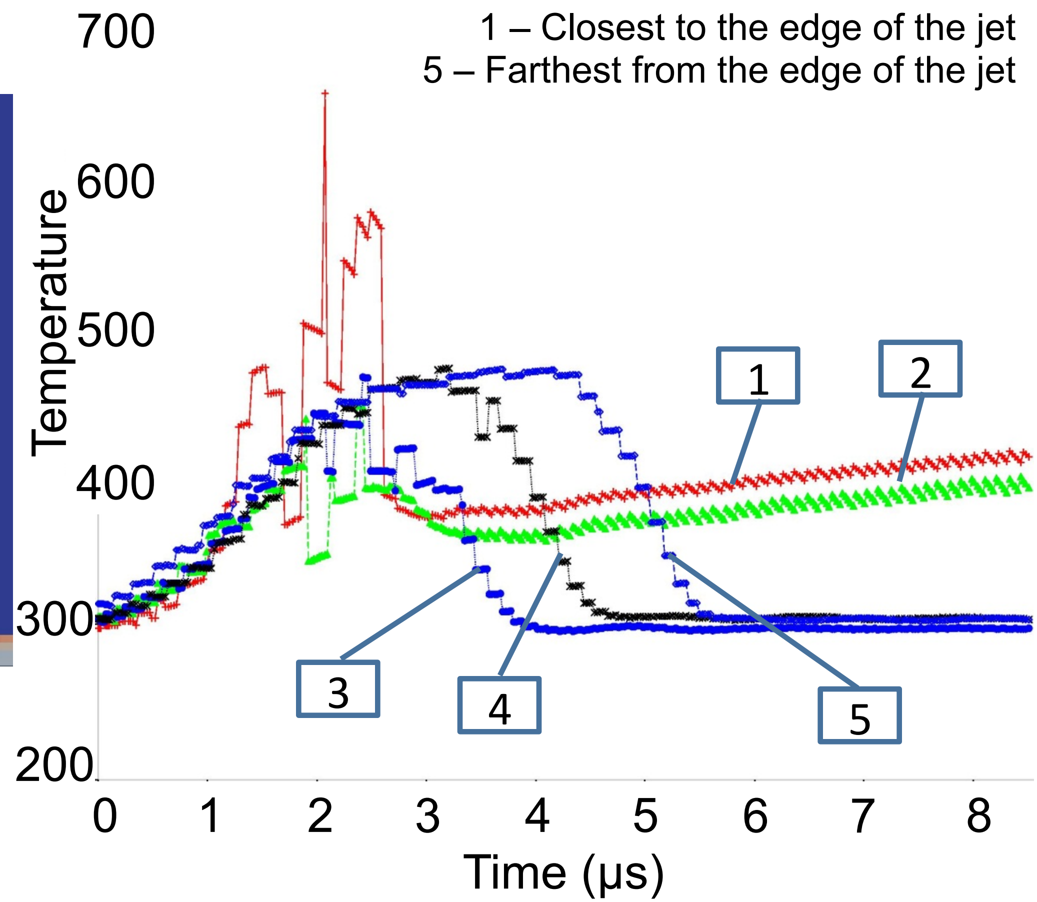


Heating Along the Jet – Under Resolved

- Default settings of artificial viscosity cause heating along the edge of the jet in under resolved cases

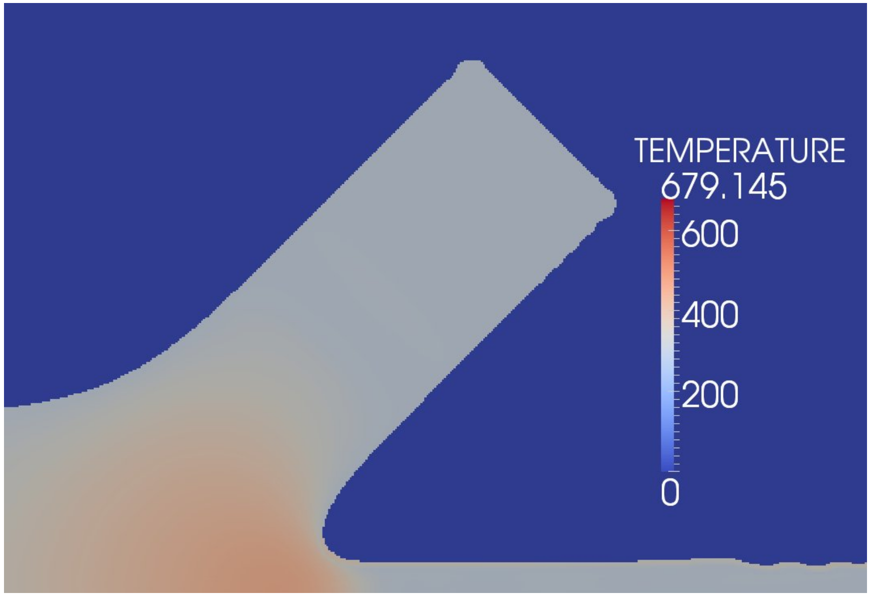


8.5 µs

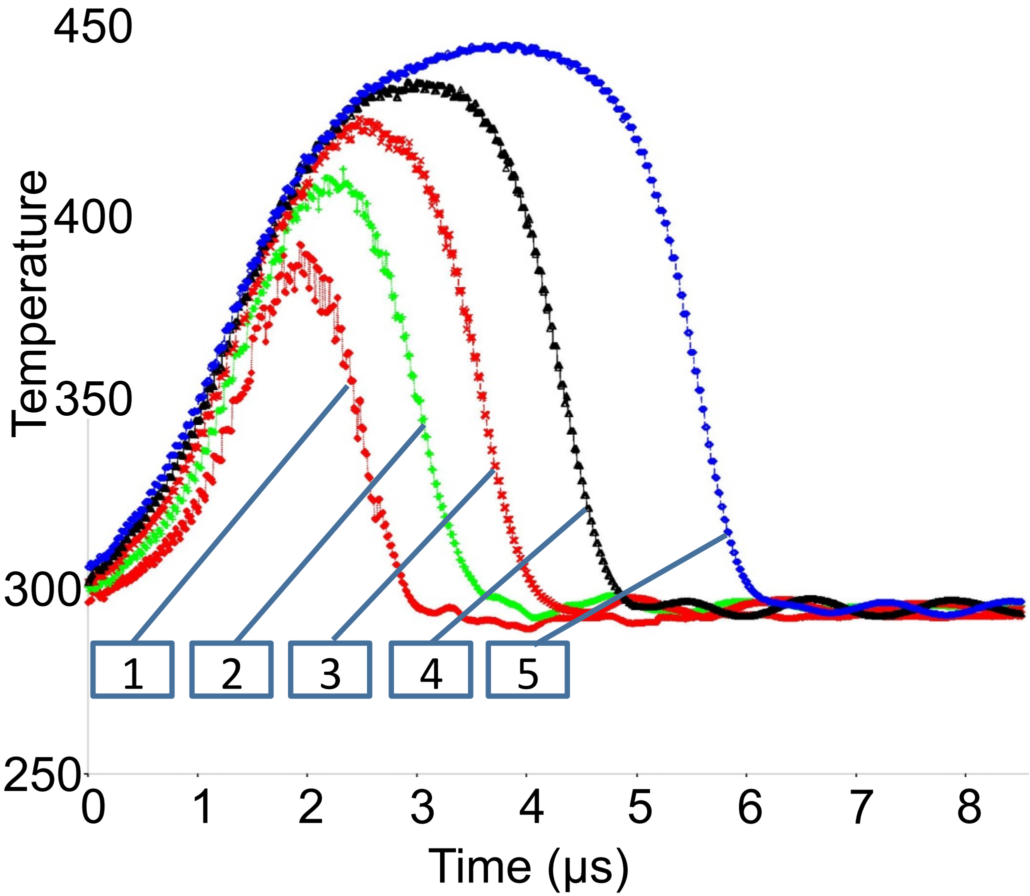


Resolution Study

A resolved mesh completely reduces the heating along the edge of the jet, results consistent with about a first-order convergence.



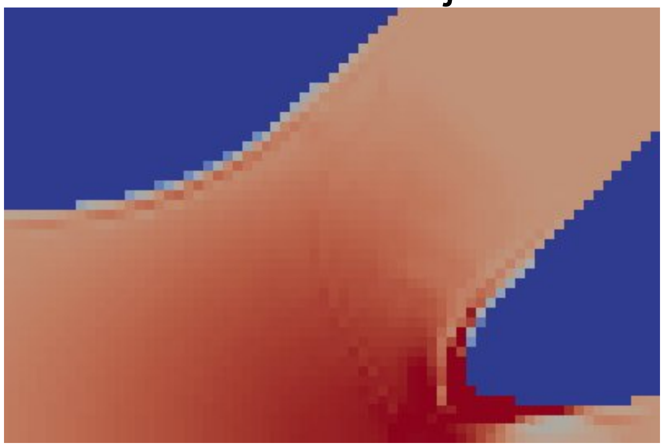
8.5 μs



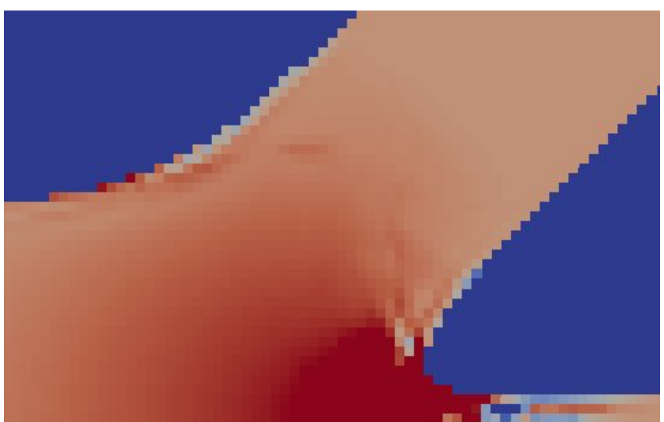
Debar Energy Advection – Resolved

Temperature irregularities are still seen with a resolved mesh

4 elements across jet

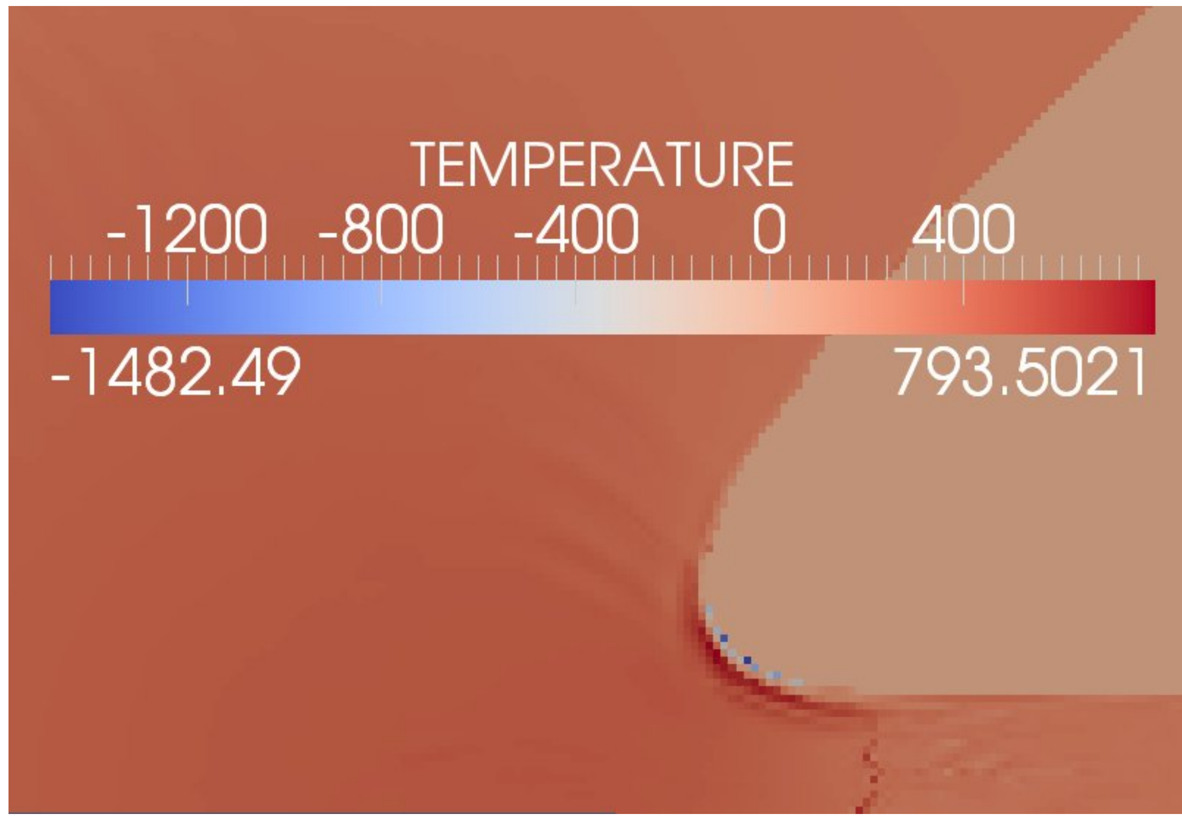


Stagnation Point Frame



Laboratory Frame

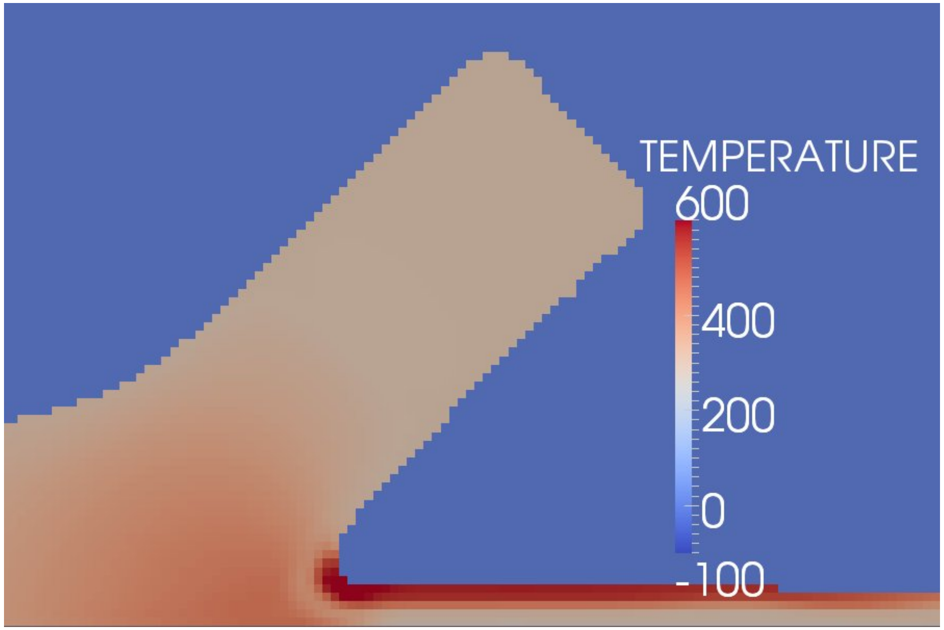
16 elements across jet

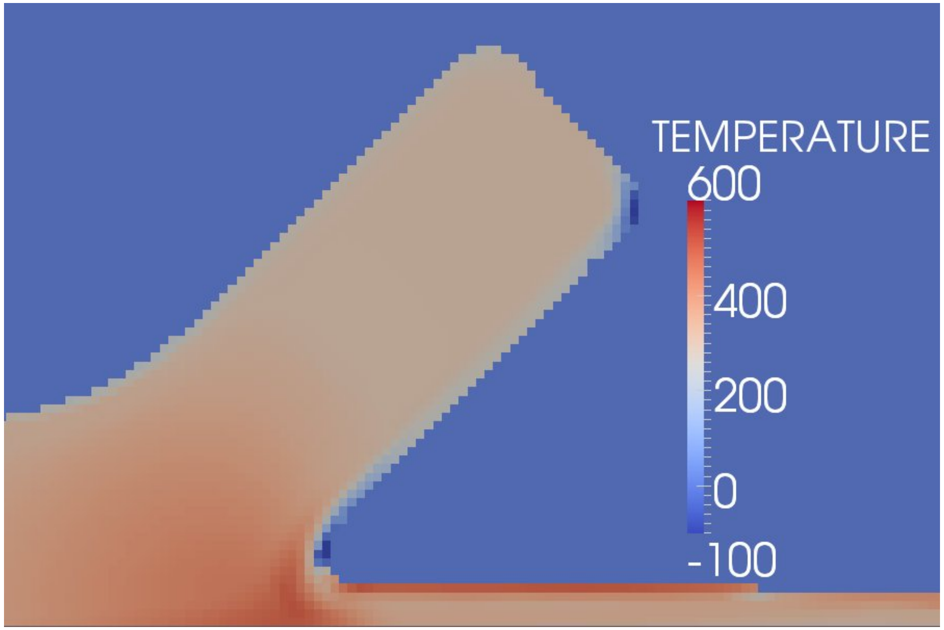


Standard Artificial Viscosity
Limiter and Hyperviscosity ON/OFF

45° Lab Frame case shown below at 8.5 μs

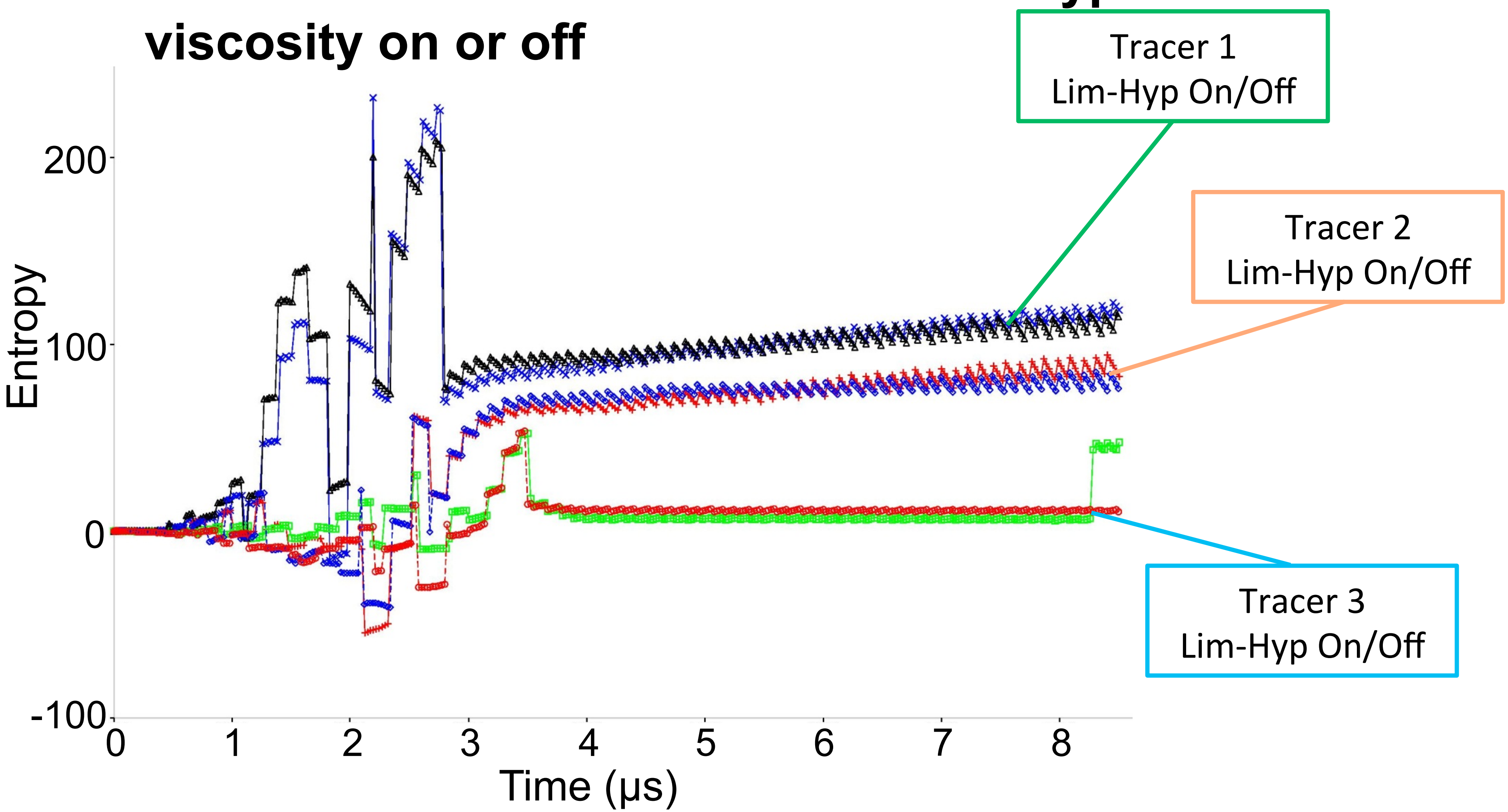
Standard Artificial Viscosity – Default Settings		Standard Artificial Viscosity – New Settings	
Linear	0.15	Linear	1.00
Quadratic	2.0	Quadratic	2.5
Expansion Linear=	OFF	Expansion Linear=	ON
Expansion Quadratic=	OFF	Expansion Quadratic=	OFF
Limiter =	OFF	Limiter =	ON
Hyperviscosity =	0.0	Hyperviscosity =	1.0





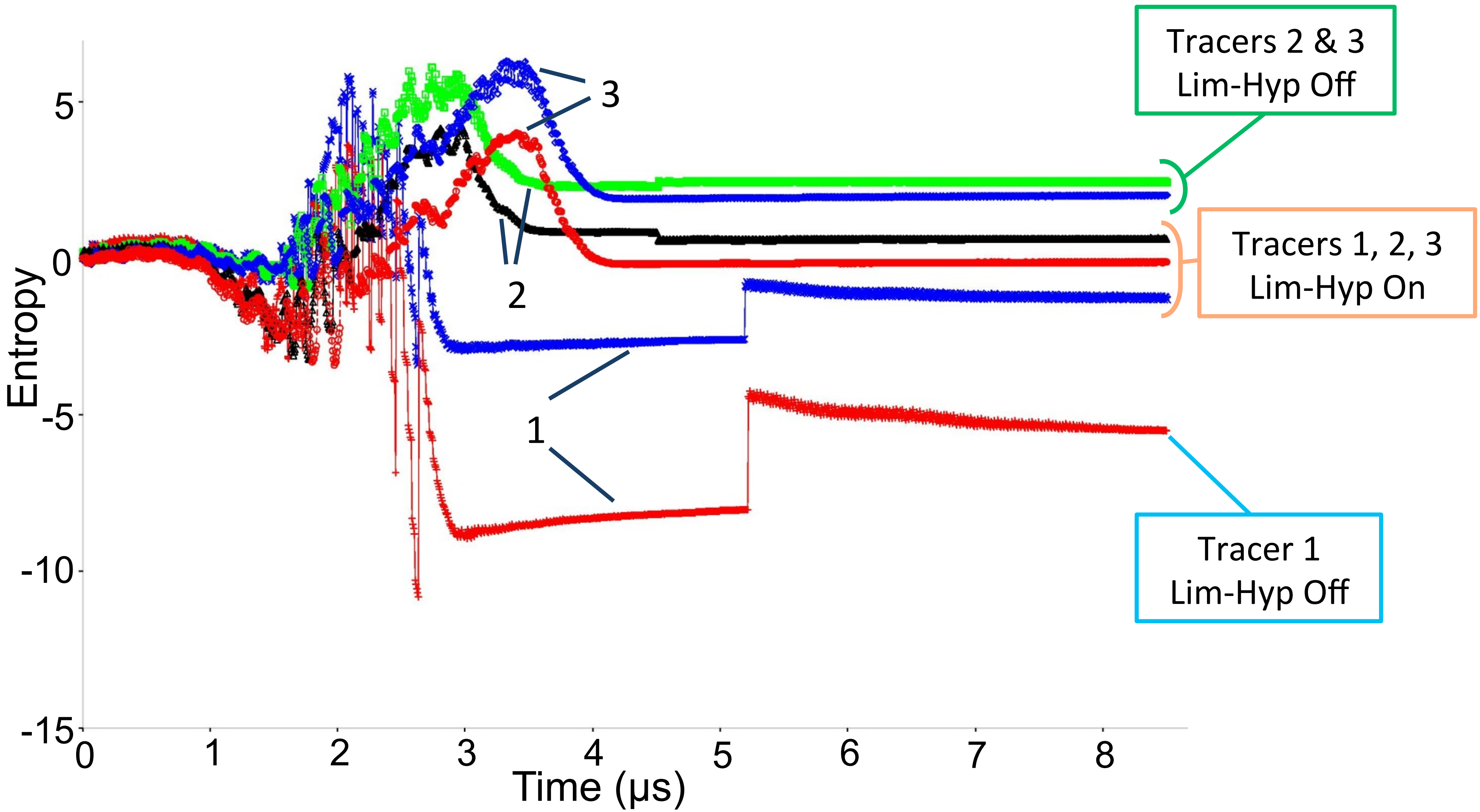
Entropy
Limiter and Hyper Viscosity ON/OFF

With low resolution, little difference is noticeable between tracers with the limiter and hyper viscosity on or off



Entropy – High Resolution
Limiter and Hyper Viscosity ON/OFF

With a resolved mesh, the limiter and hyper viscosity improve the results of the simulation



“I love to talk about nothing. It's the only thing I know anything about.”
— Oscar Wilde

Conclusions

- **Efforts to improve the modernity and resilience of the code is in mid-stream.**
- **The complexity of the effort has made it difficult**
- **The standard that we apply to code results makes changing the defaults difficult but drives a detailed look at old and new algorithms**
- **We have to balance a number of requirements:**
  - **Regression Testing Suite**
  - **Quality Embedded Verification Expectations**
  - **Prototype Problems Requirements**
  - **Customer Needs and Expectations**
  - **Performance Characteristics**

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