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ALEGRA Update: Modernization and Resilience Progress

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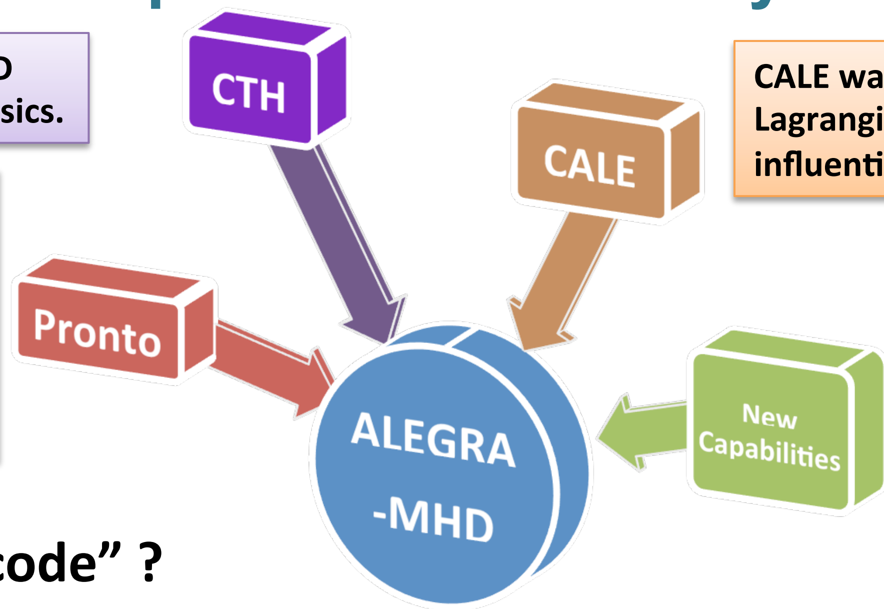
ALEGRA is a hydrocode with specific multi-physics capabilities develop over the last 20+ years.

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

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



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

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

What is a “hydrocode” ?

- A solution of the governing equations using a fluid approximation including shock physics and high-strain rate material deformation.
- Uses artificial viscosity for shocks

What key defining capabilities does ALEGRA possess?

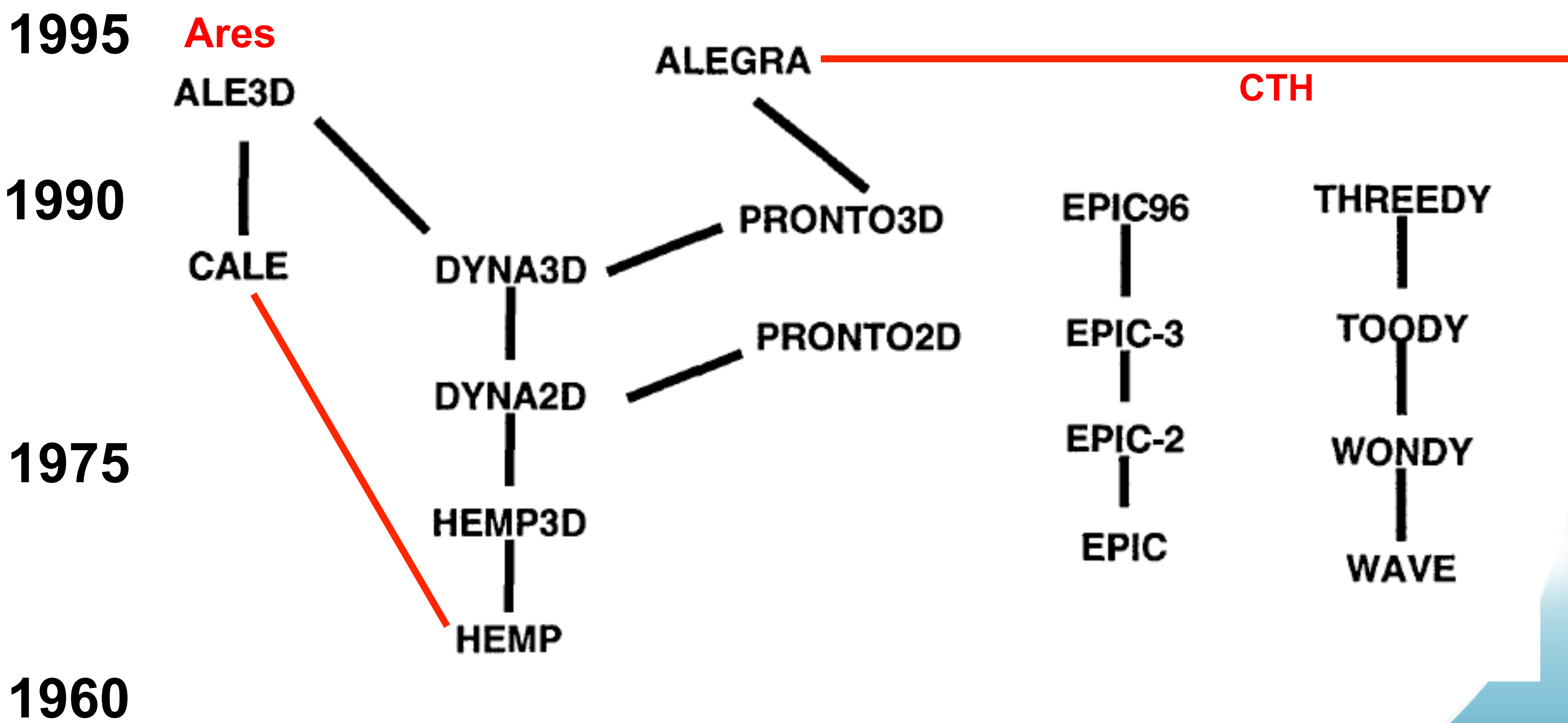
- Mimetic magneto-hydrodynamics (MHD), circuit modeling
- Extended finite element (XFEM) under development
- High fidelity material modeling (especially for MHD)
- Ceramic material models
- Optimization and UQ linkage to DAKOTA
- Robust modeling of high-strain rate deformation.

A (very) brief history of ALEGRA

- **The project began in 1988 to support the ICF program.**
- **Based on existing codes PRONTO and algorithms inspired by CTH**
- **Major support and development under the DOE ASC(I) program through the 1990's to today**
- **Developed in C++ for high-performance massively parallel computers**

"History is merely a list of surprises. It can only prepare us to be surprised yet again." – Kurt Vonnegut

SNL branch of the family tree of Lagrangian hydrocodes (by Gene Hertel, revised)



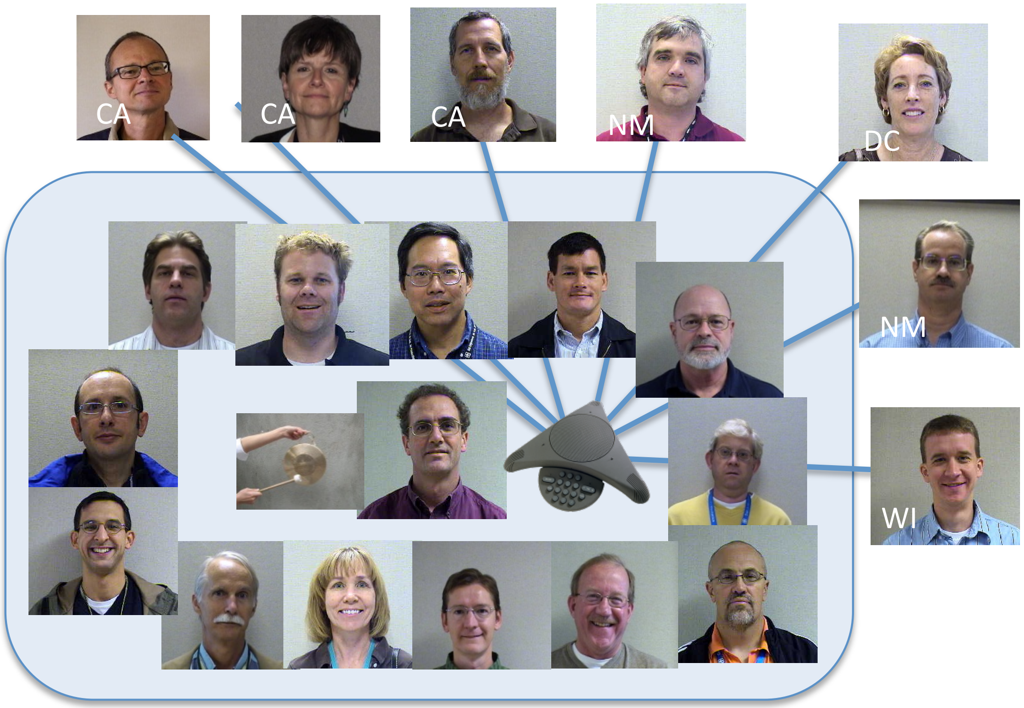
"No code is an island"

Key ALEGRA Team Members (Summer 2013)

- **1443 - Allen C. Robinson (PI) John Carpenter, Susan Carroll, Richard Drake, Chris Garasi,, David Hensinger, Chris Kueny, Duane Labreche, Edward Love, Christopher Luchini, Jay Mosso, John Niederhaus, Sharon Petney, Bill Rider, Josh Robbins, Chris Seifert, O. Erik Strack, Mike Wong, Thomas Voth, Ann Mattsson**
- **Students this summer: David Reber, David Merrell, Brad Hanks**
- **Other 1400: V. Greg Weirs, Tim Trucano, Brian Adams, Dena Vigil, Curt Ober, Randy Summers, Jim Stewart, Pavel Bochev**
- **1600/1641: Thomas Haill, Ray Lemke, Mike Desjarlais, Kyle Cochrane, Thomas Mattsson**
- **LANL: John Walter, Kristi Brislawn**

Our solution to historical delivery challenges is to take an integrated approach to code development.

- **We address short comings in four areas:**
  - physical modeling,
  - numerical algorithms,
  - code development attitudes,
  - code development practices.
- **We strive to build a tightly knit team**
  - 15 minutes daily standup meeting ,
  - fast cycle for project planning
  - Automated testing with user prototype, verification & performance suites. Verification tests are the expected norm above and beyond simple regression testing.



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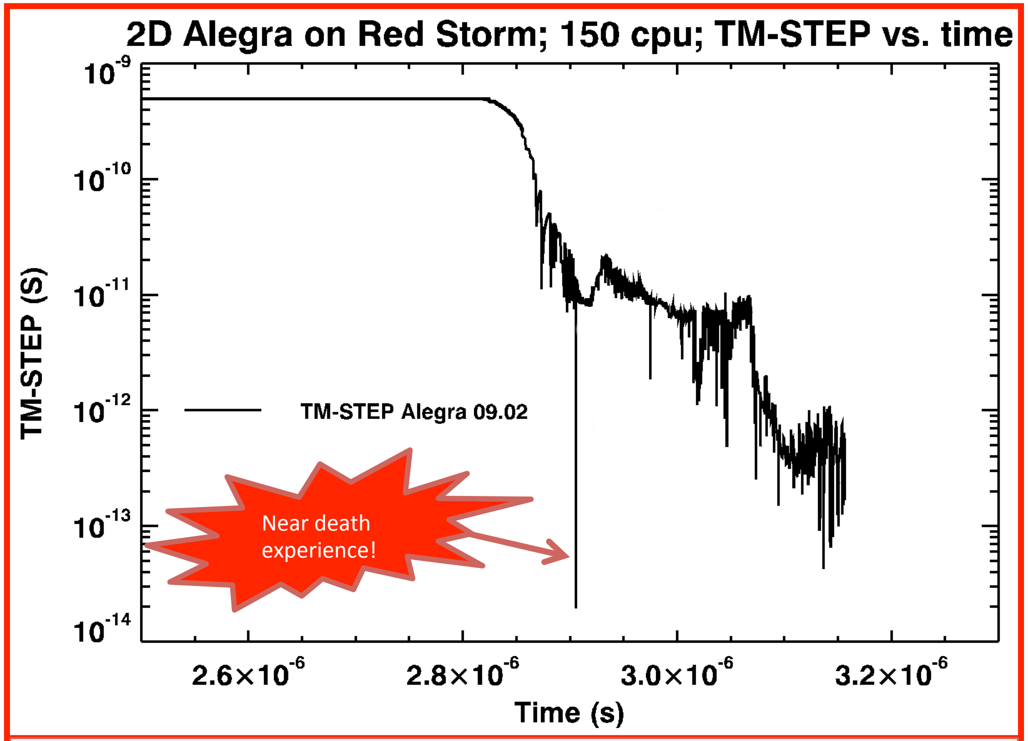
Looking back in time sets the stage for this year's efforts.

Previous success is attempted to be recreated!

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.

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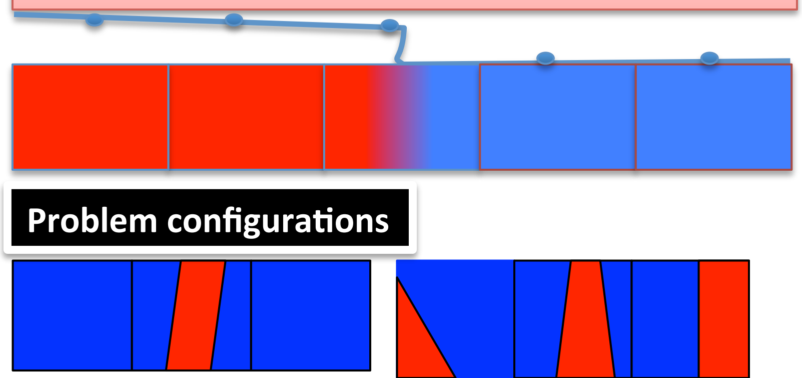
We made improvements in the remap and multimaterial methods plus the stability criteria.

Summary of remap changes: Detect the local multimaterial flow topology



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

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

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

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

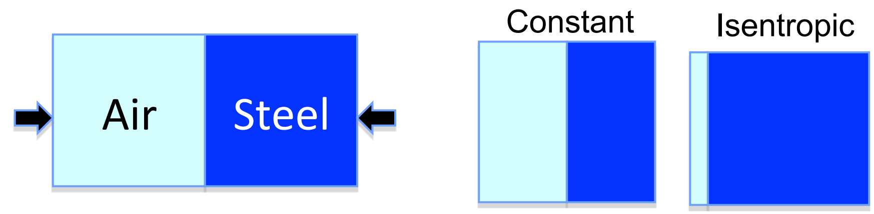
Mixed cell remap is now lower order

- **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



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

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

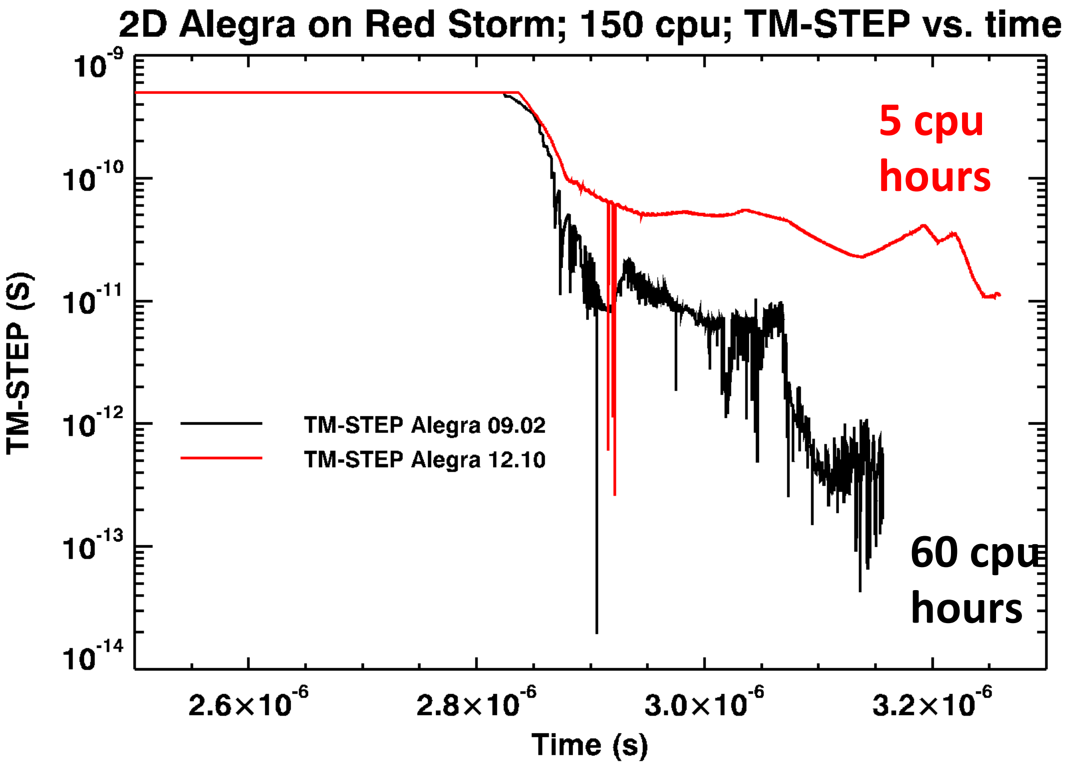
Summary of time step size calculations: based upon the Fourier analysis of the Lagrangian step with dissipation.

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

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!

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Based on our success, we have engaged in taking the next steps forward.

Modern Artificial Viscosity: Use the velocity Laplacian to limit the artificial viscosity

- A linear velocity field is smooth, does not represent a shocked flow, and also has zero Laplacian.
- Computation of the velocity Laplacian

$$(\nabla^2 \mathbf{v}) = \nabla(\nabla \cdot \mathbf{v}) - \nabla \times (\nabla \times \mathbf{v}) = \mathrm{div}[\mathrm{grad}[\mathbf{v}]]$$

$$\int_\Omega \boldsymbol{\eta} \bullet (\nabla^2 \mathbf{v})\, \mathrm{d}\Omega \;=\; -\int_\Omega \mathrm{grad}[\boldsymbol{\eta}] \bullet \mathrm{grad}[\mathbf{v}]\, \mathrm{d}\Omega \;+\; \int_{\partial\Omega} \boldsymbol{\eta} \bullet \mathrm{grad}[\mathbf{v}]\, \mathbf{n}\, \mathrm{d}\Gamma \quad \forall \boldsymbol{\eta}$$

$$\theta_A \;=\; \frac{\left\| -\int_{\Omega_A} \mathrm{grad}[\mathbf{v}]\mathrm{grad}[N^A] + \boxed{\int_{\partial\Omega_A} \mathrm{grad}[\mathbf{v}] N^A \mathbf{n}} \right\|}{\int_{\Omega_A} \|\mathrm{grad}[\mathbf{v}]\mathrm{grad}[N^A]\| + \boxed{\int_{\partial\Omega_A} \|\mathrm{grad}[\mathbf{v}] N^A \mathbf{n}\|}} \;\leq\; 1$$

General structure of an improved artificial viscosity has several elements

- **High-order "flux" is "zero artificial viscosity".**
- **Low-order "flux" is "standard artificial viscosity".**
- **Limited artificial viscosity if** $\mathrm{trace}[\mathbf{d}] < 0.0 \qquad \mathbf{d} = \mathrm{grad}^s[\mathbf{v}]$

$$\boldsymbol{\sigma}_{art}^{LO} = \rho \left[c_1 \, c \, h \; + \; c_2 \, \|\mathrm{trace}[\mathbf{d}]\| \, h^2 \right] \mathbf{d}$$

$$\boldsymbol{\sigma}_{art} = \theta \boldsymbol{\sigma}_{art}^{LO}$$

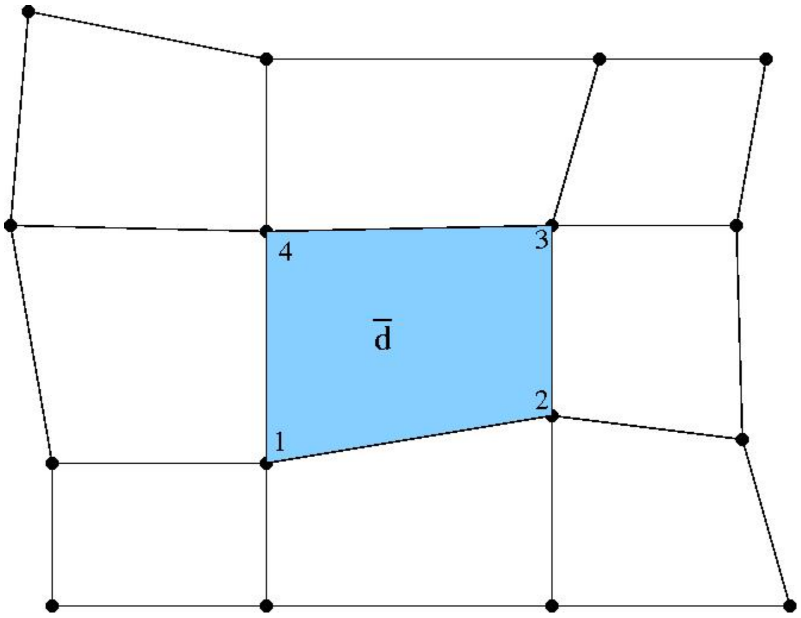
- **If the velocity field is linear, then the artificial viscosity is zero on both the interior and the boundary of arbitrary unstructured meshes.**
- **Important to include boundary terms (red boxed terms on previous slide).**

HyperViscosity can be developed by filtering the second-order viscosity.

- **Define $\bar{\mathbf{d}}$ as the mean rate of deformation over a patch of elements.**

$$\Omega_{patch} = \bigcup_{A=1}^{4} \mathrm{supp}(N^A)$$

$$\bar{\mathbf{d}} = \frac{1}{\mathrm{meas}(\Omega_{patch})} \int_{\Omega_{patch}} \mathbf{d} \, \mathrm{d}\Omega$$



- **Add additional viscosity**

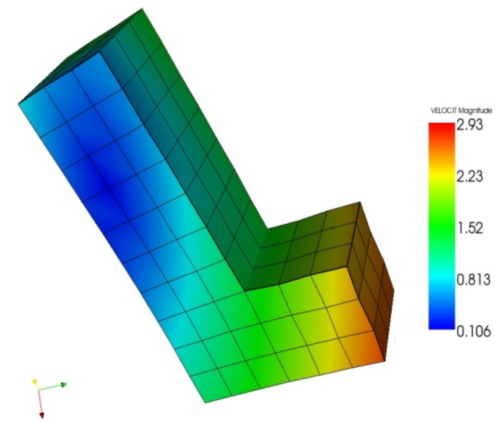
$$\boldsymbol{\sigma}_{hyper} = c_3 \left[\boldsymbol{\sigma}^{LO}_{art}(\mathbf{d}) - \boldsymbol{\sigma}^{LO}_{art}(\bar{\mathbf{d}}) \right]$$

$$\boldsymbol{\sigma}_{art} = \theta \boldsymbol{\sigma}^{LO}_{art}(\mathbf{d}) + (1-\theta)\boldsymbol{\sigma}_{hyper}$$

- **The hyperviscosity also vanishes for a linear velocity field since in that case $\mathbf{d} = \bar{\mathbf{d}}$.**

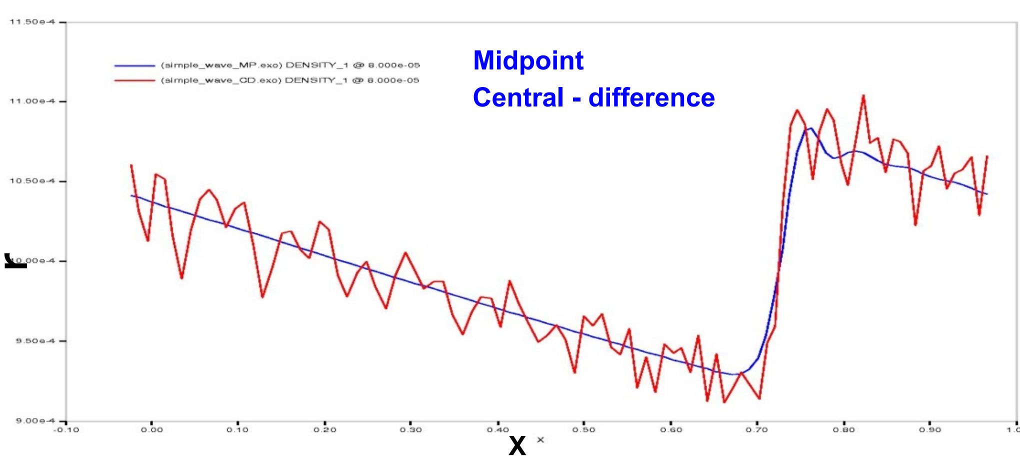
Improved Time Integration Algorithms through the midpoint method.

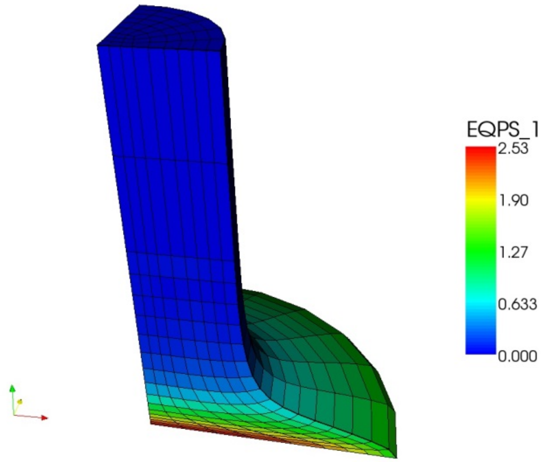
- *Central-difference* method is *unconditionally unstable* (w/o Q).
- Midpoint predictor-corrector is stable.
- Predictor-corrector is exactly energy conservative.
- Predictor-corrector is 2^{nd}-order accurate.
- Support for solid models is in progress.
- Rotation interpolation using the exponential map.



$$\bar{\mathrm{q}} = \frac{\sin(\theta/2)}{\sin(\theta)}(\mathrm{q}_0 + \mathrm{q}_1) = \frac{1}{2\cos(\theta/2)}(\mathrm{q}_0 + \mathrm{q}_1) \qquad \cos(\theta) = \mathbf{q}_0 \bullet \mathbf{q}_1$$

- Periodic breaking wave problem confirms theoretical results.





Default Time integration method: Centered Difference

- The method is basically an explicit leapfrog method (central difference scheme).
- Velocity and RoD are at the half-time level (n +1/2), $\vec{a} = \vec{u}_t$

$$\vec{u}^{n+1/2} = \vec{u}^{n-1/2} + \tfrac{1}{\rho}\Delta t \nabla^n \cdot \sigma^n$$

- Other quantities are at the full-time level (n),

$$\vec{x}^{n+1} = \vec{x}^n + \Delta t \vec{u}^{n+1/2}$$

- Everything is second-order w/o Q or the energy equation, which is first order with.

$$e^{n+1} = e^n + \Delta t \sigma^n \bullet \nabla^n \left(\tfrac{1}{2}\vec{u}^{n-1/2} + \tfrac{1}{2}\vec{u}^{n+1/2} \right)$$

New Time integration method: Midpoint

- **The method is basically a predictor-corrector modified to be conservative.**
- **Quantities are predicted at the full-time level (n+1),**

$$\tilde{u} = u^n - \Delta t \nabla_m \left(p^n + q^n \right) \qquad \tilde{x} = x^n + \Delta t \left(\tfrac{u^n + \tilde{u}}{2} \right)$$

$$\tilde{e} = e^n - \Delta t \left(p^n + q^n \right) \nabla_m \cdot \left(\tfrac{u^n + \tilde{u}}{2} \right) \qquad \tilde{p} = \mathrm{P}\left(\tilde{\rho}, \tilde{e} \right)$$

- **This allows a centered corrector step.**

$\tilde{p} \rightarrow p^{n+1}$

$$u^{n+1} = u^n - \Delta t \nabla_m \left(\frac{p^n + q^n + \tilde{p} + \tilde{q}}{2} \right)$$

$$x^{n+1} = x^n + \Delta t \left(\frac{u^n + u^{n+1}}{2} \right)$$

$$e^{n+1} = e^n - \Delta t \left(\frac{p^n + q^n + \tilde{p} + \tilde{q}}{2} \right) \nabla_m \cdot \left(\frac{u^n + u^{n+1}}{2} \right)$$

$$p^{n+1} = \mathrm{P}\left(\rho^{n+1}, e^{n+1} \right)$$

Could do multiple iterations

- **Everything is second-order w/o Q and could be iterative with the nonlinear EOS.**

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Improved Constrained Transport of Magnetic Flux

$$\begin{aligned}\mathbf{B}(\xi_1,\xi_2,\xi_3) &= \Phi_1^+(\xi_2,\xi_3)\mathbf{W}_1^+ + \Phi_1^-(\xi_2,\xi_3)\mathbf{W}_1^- + \\ &\quad \Phi_2^+(\xi_3,\xi_1)\mathbf{W}_2^+ + \Phi_2^-(\xi_3,\xi_1)\mathbf{W}_2^- + \\ &\quad \Phi_3^+(\xi_1,\xi_2)\mathbf{W}_3^+ + \Phi_3^-(\xi_1,\xi_2)\mathbf{W}_3^-\end{aligned}$$

$$\Phi_i^+(\xi_2,\xi_3) = \Phi_i^+ + s_{i2}^+\xi_2 + s_{i3}^+\xi_3$$

Use least square representation at nodes to compute s values at nodes

$$\begin{aligned}4\det J_F(p) \quad \mathbf{B}(p) = \quad & \Phi_1^+(1,0)\mathbf{V}_1(p) + \\ & \Phi_2^+(0,1)\mathbf{V}_2(p) + \\ & (\Phi_3^+(1,1)+\Phi_3^-(1,1))\mathbf{V}_3(p)\end{aligned}$$

$$\begin{aligned}4\mathbf{B}(p)\cdot(\mathbf{V}_2(p)\times\mathbf{V}_3(p)) &= \Phi_1^+(1,0) \\ 4\mathbf{B}(p)\cdot(\mathbf{V}_3(p)\times\mathbf{V}_1(p)) &= \Phi_2^+(0,1)\end{aligned}$$

Limit (harmonic limiting)

$$\begin{aligned}s_{12}^+ &= 2s_{12}^{++}s_{12}^{+-}/(s_{12}^{++}+s_{12}^{+-}),\ \mathrm{if} s_{12}^{++}s_{12}^{+-} > 0 \\ s_{12}^+ &= 0,\ \mathrm{otherwise}\end{aligned}$$

Edge integration

$$\hat{\xi}_i = \frac{\delta\xi_i}{2} + \xi^{ec}$$

$$\begin{aligned}\int_S \mathbf{B}\cdot d\mathbf{a} \approx & \frac{1}{4}(-\Phi_2^+(\hat{\xi}_3,\hat{\xi}_1)(1+\hat{\xi}_2) - \Phi_2^-(\hat{\xi}_3,\hat{\xi}_1)(1-\hat{\xi}_2))\delta\xi_1 \\ & + \frac{1}{4}(\Phi_1^+(\hat{\xi}_2,\hat{\xi}_3)(1+\hat{\xi}_1) + \Phi_1^-(\hat{\xi}_2,\hat{\xi}_3)(1-\hat{\xi}_1))\delta\xi_2\end{aligned}$$

DeBar correction

ALEGRA uses a modern implementation of DeBar's correction for the kinetic energy loss arising in elements near shocks due to remap:

conservatively remapped KE — actual remapped KE

$$\Delta E_k = \frac{1}{N}\sum_{n=1}^{N}\frac{1}{2}\mathcal{R}[m](\mathcal{R}[\mathbf{v}_n]\cdot\mathcal{R}[\mathbf{v}_n]) - \mathcal{R}\left[\frac{1}{N}\sum_{n=1}^{N}\frac{1}{2}m(\mathbf{v}_n\cdot\mathbf{v}_n)\right]$$

$$E_i^{\mathrm{DeBar}} = E_i + \Delta E_k$$

$\mathcal{R}[.]$ = remap operator

m = mass associated with element

$\mathbf{v}_n$ = nodal velocity

The traditional form of the DeBar correction maintains full conservation of energy in remap for pure hydrodynamics.

Optional limiters are included in the implementation:

- Restrict to shocks only, using value of Q/P
- Limit magnitude of correction in the case of cooling

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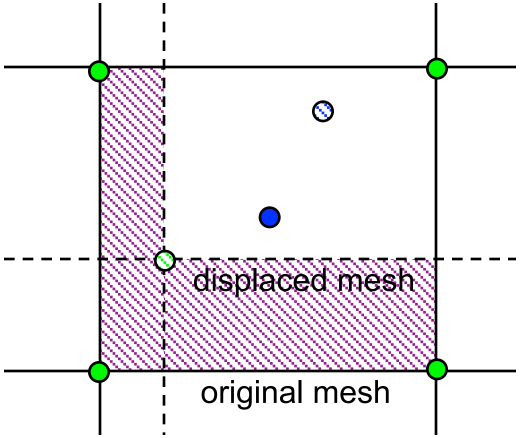
Magnetic energy is also lost in LR schemes for MHD

Remap of magnetic variables can be introduced using constrained transport*

- Advects magnetic flux conservatively
- Maintains divergence-free nature of the **B** field $(\nabla \cdot \mathbf{B} = 0)$



Magnetic energy is not conserved

$$E = \rho\varepsilon + \rho|\mathbf{V}|^2/2 + |\mathbf{B}|^2/2\mu$$

IE KE ME

- Magnetic flux is linear in **B**, but ME is quadratic
- Magnetic fluxes represented at **faces**, but internal energies at **element centers**

→ **Only IE is remapped conservatively, and KE and ME are both not conserved**

Variables conservatively advected in remap:

Mass, momentum, internal energy, and magnetic flux

*Evans and Hawley, *Ap. J.*, 1988

DeBar correction: A method for restoring energy conservation in LR schemes

DeBar (1974) first proposed a simple correction to address this issue:

- Remap kinetic energy independently
- Compute discrepancy relative to KE arising from remapped mass and momentum
- Eliminate the discrepancy by adding it to the remapped IE

$$\Delta E_k = \frac{1}{2}\frac{1}{\mathcal{R}[\rho]}\mathcal{R}[\rho\mathbf{V}]\cdot\mathcal{R}[\rho\mathbf{V}] - \mathcal{R}\left[\frac{1}{2}\rho\mathbf{V}\cdot\mathbf{V}\right]$$

$\mathcal{R}[.]$ = remap operator

Allen Robinson has extended the DeBar correction for MHD:

$$\Delta E_m = \frac{1}{2\mu}\mathcal{R}[\mathbf{B}]\cdot\mathcal{R}[\mathbf{B}] - \frac{1}{2\mu}\mathcal{R}[\mathbf{B}\cdot\mathbf{B}]$$

Magnetic DeBar correction is implemented in ALEGRA, <u>needs verification</u>

- Hydrodynamic DeBar correction has been implemented in numerous codes (ALEGRA, ALE3D, ARES, CTH, FLAG, TURMOIL3D)
- Issues: solution uniqueness, code robustness.
- ALEGRA is the first LR code with the MHD DeBar correction (full energy conservation in MHD)

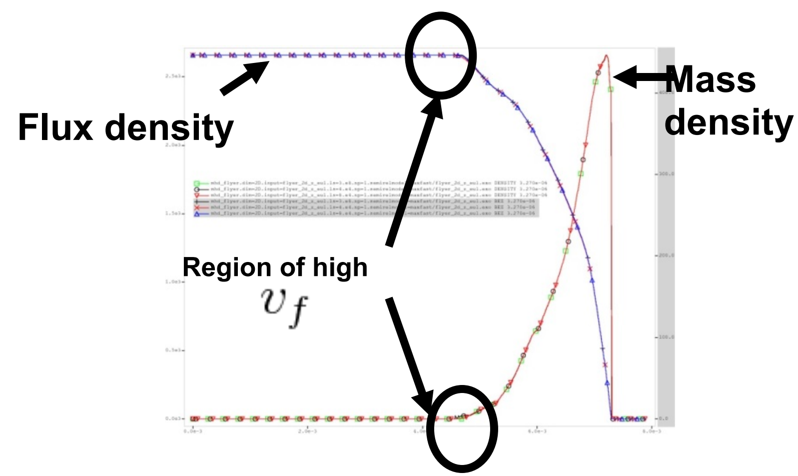
The Boris Correction: aka “maxfast”

$$\frac{d}{dt}\int (1+\frac{v_A^2}{c^2})\rho\mathbf{v}dv = \int \nabla\cdot(-p\mathbf{I}) + \nabla\cdot\left(\frac{1}{\mu_0}\mathbf{B}\otimes\mathbf{B} - \frac{1}{2\mu_0}B^2\mathbf{I}\right)dv$$

Mass multiplier

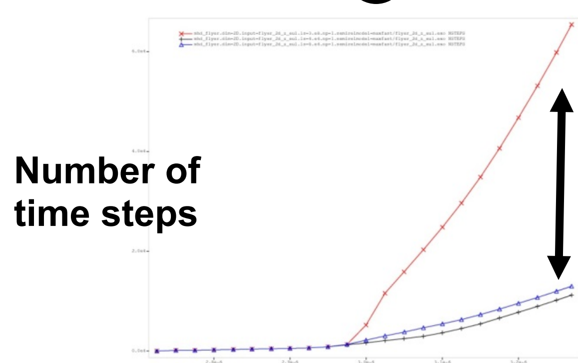
$$v_f^2 = \frac{a^2+v_A^2}{1+(v_A/c)^2}$$

3.e8, 80.e3, 40e3 km/s



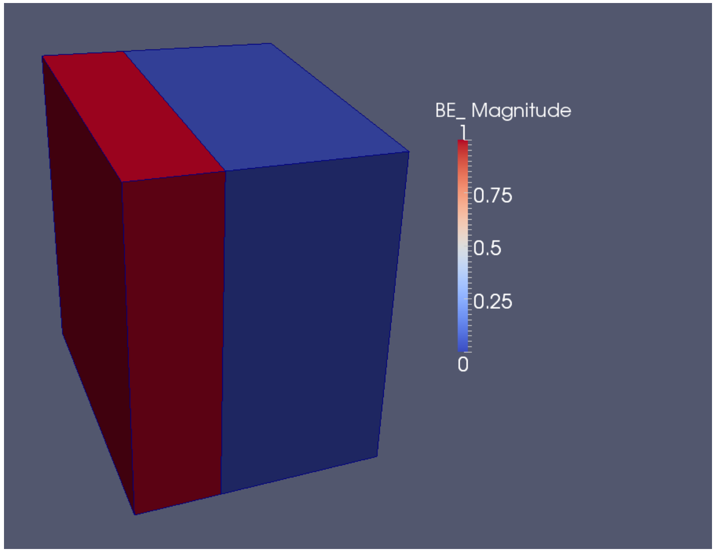
- The maximum fast speed is reduced by the square root of the inverse mass multiplier.
- Using the true light speed in the mass multiplier will have no benefit. In order to reduce the overall impact on the physics, the correction should be applied only where the fast speed is too large.

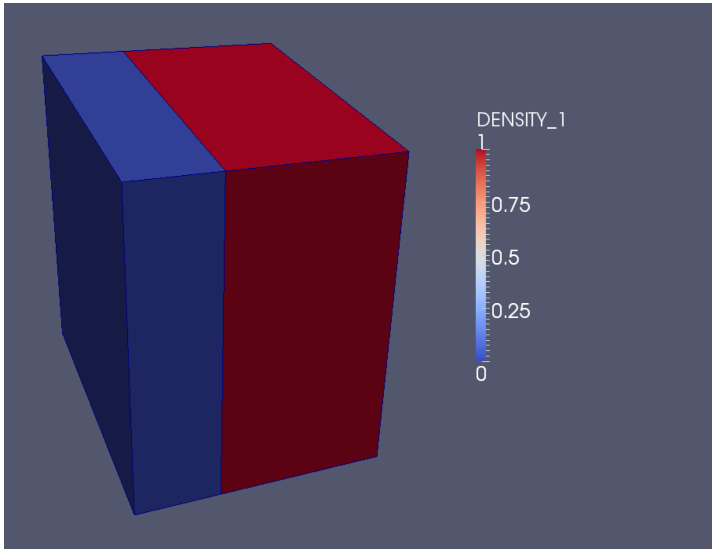
$$v_f = \min\left(1, \frac{v_f^{max}}{\sqrt{a^2+v_A^2}}\right)\sqrt{a^2+v_A^2} = \alpha\sqrt{a^2+v_A^2}$$



- Reduce accelerations by a factor proportional to a^2
- The algorithm essentially compute a beneficial spatially varying “light speed”.

An improved time step estimate for material/void interfaces with magnetic field is necessary.





- Test problem: two elements; one void with magnetic field; one ideal gas zero magnetic field;
- Initial static equilibrium (physical pressure = magnetic pressure).
- Unstable at CFL=0.90 for this problem (static equilibrium not preserved).
- Time step calculation does not account for “stiffness” of void element.
- Lagrangian “stiffness” comes from coupling of momentum and induction equations.
- Possible fix: add in neighbor’s magnetic field(s) during Alfven wave speed calculation.

$$\omega^2 = 2\left[h_1^{-1} h_2^{-1} \rho^{-1} \frac{1}{\mu_0} B_y^2 + h_2^{-2} c^2 \right]$$

Extra Term

Expected Term

Nodal Force Limiter

- **We have noted that the nodal forces may sometimes be too large for stability, and an additional test may remove the instabilities.**
- **This is shown to be directly associated with several key code resilience issues.**
- **The analysis of the problem revealed two issues that are presently unresolved.**
  - ALEGRA time step control may not be strict enough because of the length scale chosen in time step determination.
  - The nodal force limiter's form may not be adequete.
- **We need to implement the changes and reassess.**

$$F \leq Cm_{node} \Delta x / \Delta t^2 \rightarrow Cm_{node} \left(c_s + \Delta x / \Delta t \right) / \Delta t$$

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Resilience: Nodal Force Limiter

- We dealt with all the fails except emission2T.
- The analysis of the problem revealed two issues that are presently unresolved.
  - ALEGRA time step control may not be strict enough because of the length scale chosen in time step determination.
  - The nodal force limiter's form may not be adequate. $F \leq Cm_{node} \Delta x / \Delta t^2 \rightarrow Cm_{node} \left(c_s + \Delta x / \Delta t \right) / \Delta t$
- We need to implement the changes and reassess.

Code resilience: revisiting maxsigma

Treatment of Joule heating in multimaterial elements (Siefert writeup 1/4/2013):

joule heat, standard
$\widehat{P} = \int_\Omega \sigma_A \mathbf{E}\cdot\mathbf{E}\, d\Omega$ $\widehat{P}_i = \sigma_i v_i \int_\Omega \mathbf{E}\cdot\mathbf{E}\, d\Omega$

DEFAULT

joule heat, maxsigma
$\widetilde{P} = r\sigma_A \int_\Omega \mathbf{E}\cdot\mathbf{E}\, d\Omega$ $\widetilde{P}_i = r\sigma_i v_i \int_\Omega \mathbf{E}\cdot\mathbf{E}\, d\Omega$

OPTIONAL

$$\sigma_A = \sum_{i=1}^n v_i \sigma_i$$

$$r = \left(\frac{\sigma_A}{\sigma_{max}}\right)^2$$

- Anecdotal evidence shows use of maxsigma can increases resilience, especially against element inversion but is ad hoc and can give the wrong solution.
- In 2D Az formulation for spatially constant electric field the standard option is exactly correct. Can we do better?
- Kramer, Reber, Siefert, Robinson are revisiting the formulation and implementation to determine if better partitioning methods are available which make use of interface information. Results are encouraging and may point the way for other formulations and 3D.

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Code resilience work: limiter testing

Extensive testing was carried out on the contracting ring problem (Prototype/mhdrobustness2012/contractring2d) using limiters devised by Rider:

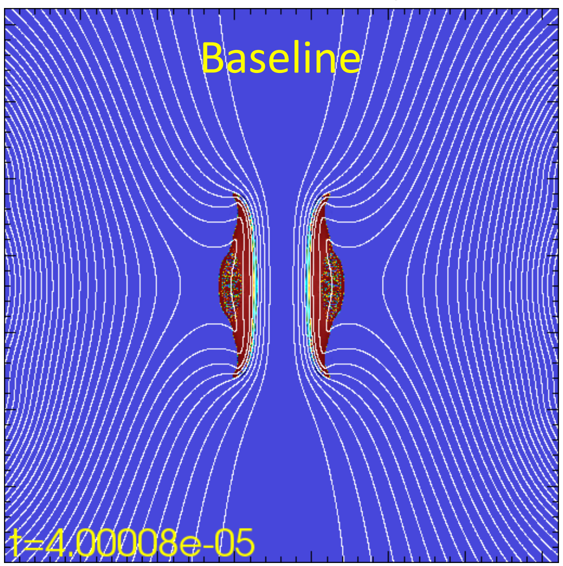
Run to completion at all mesh resolutions:

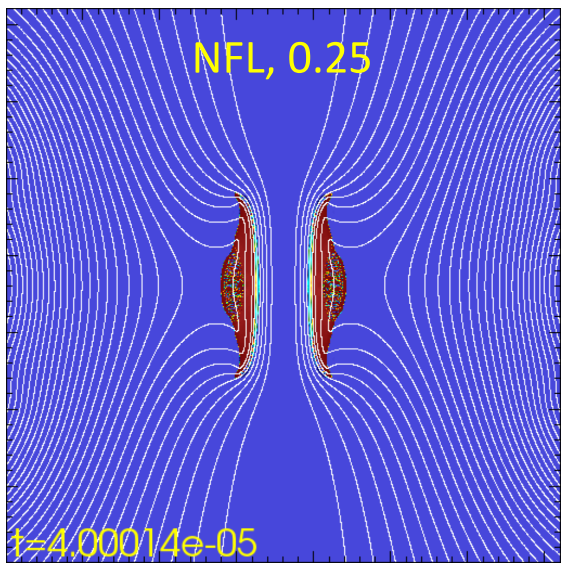
- NFL + midpoint + limiter/hypervisc
- NFL + kandc sesame + FF

Still encounter element inversion:

- VL, VV
- Debar
- Air 5032
- kandc/FF alone
- Midpoint alone
- ZNM drift velocity scale
- NFL alone

Solutions are nearly identical





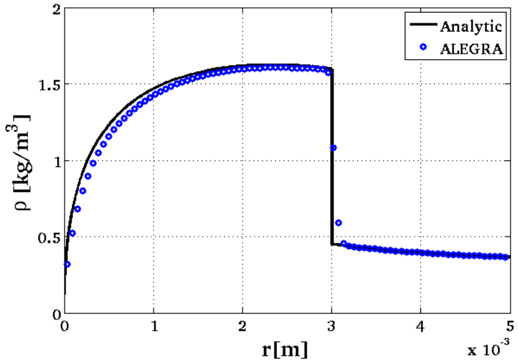
NFL = node max force limiter
VV, VL = void limiter, void viscosity options for art visc
ZNM = zero node mass
FF = force fracture

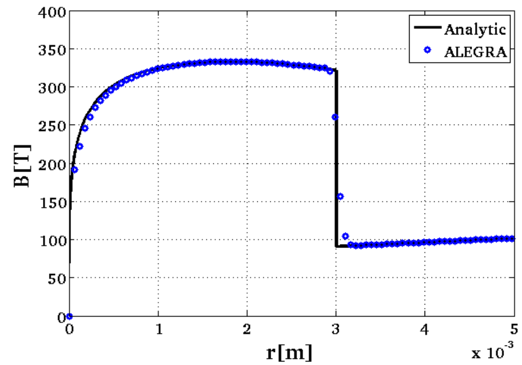
Not avail-able in trunk (yet?)

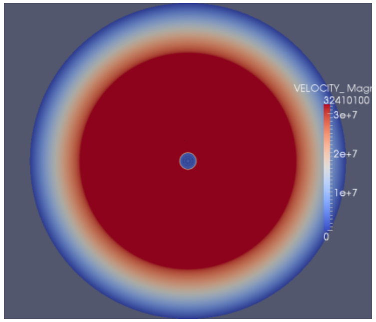
All tests used maxsigma.

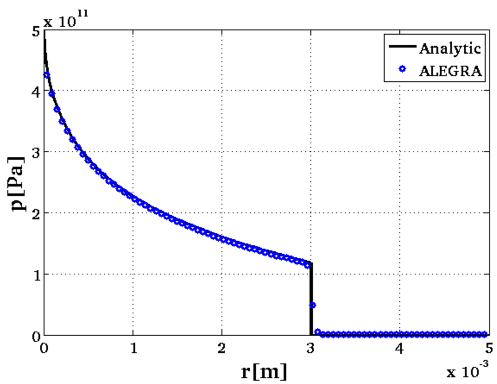
Code resilience: verification testing

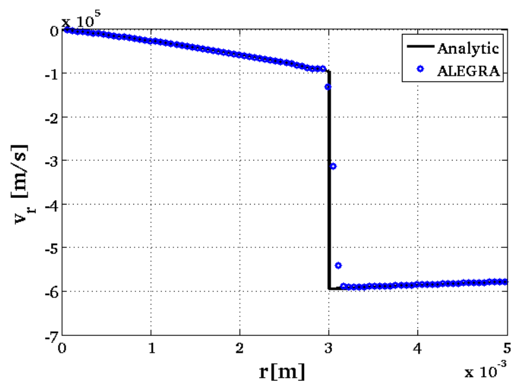
- Velikovich *et. al*. derived self-similar solutions for magnetized cylindrical Noh problem
- We are comparing to 1d radial and 2d r-q simulations with ALEGRA
- Testing new 2D magnetic Debar capability
- R, B_q, v_r and p show good agreement (3cm cylinder, 512 cells, no Debar):











Velocity profile in developing shock

Code resilience: verification testing

Verification for cylindrical magnetized Noh

- Velikovich *et. al*. derived family of self-similar solutions, and compared to Mach2 (2d r-z) and Athena (2d x-y).
- We are verifying ALEGRA in 2d and 3d against these solutions.

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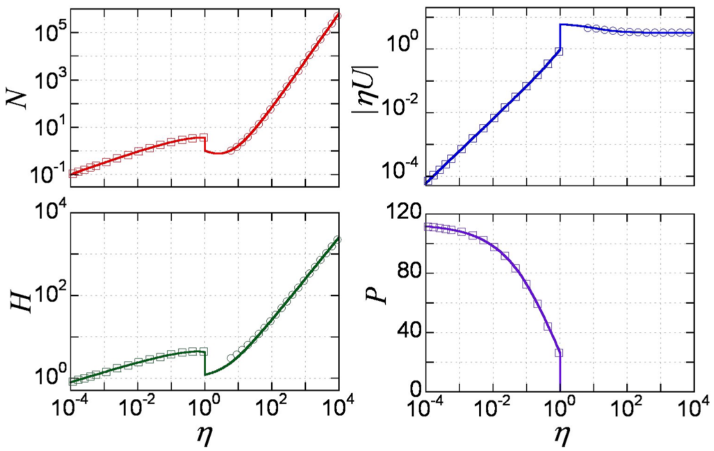
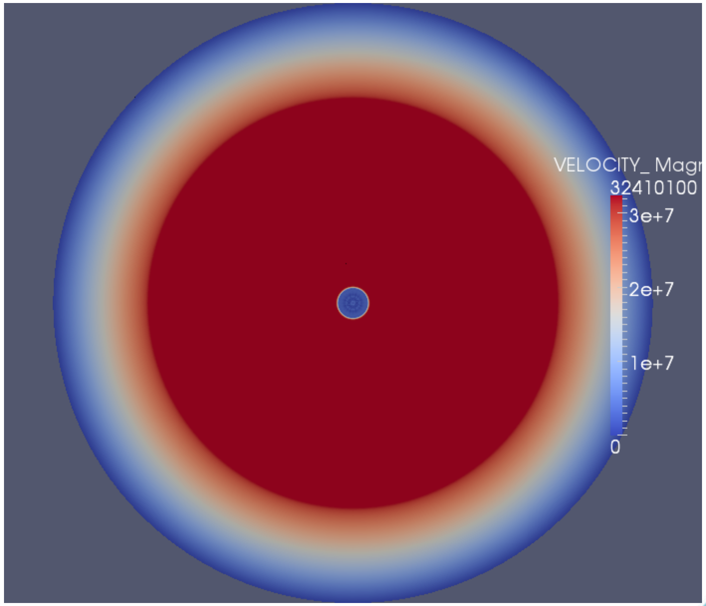


FIG. 1. (Color online) Self-similar profiles of density, velocity, magnetic field, and pressure. Line—exact solution, boxes—asymptotic expansion at $\eta \ll 1$, and circles—asymptotic expansion at $\eta \gg 1$.



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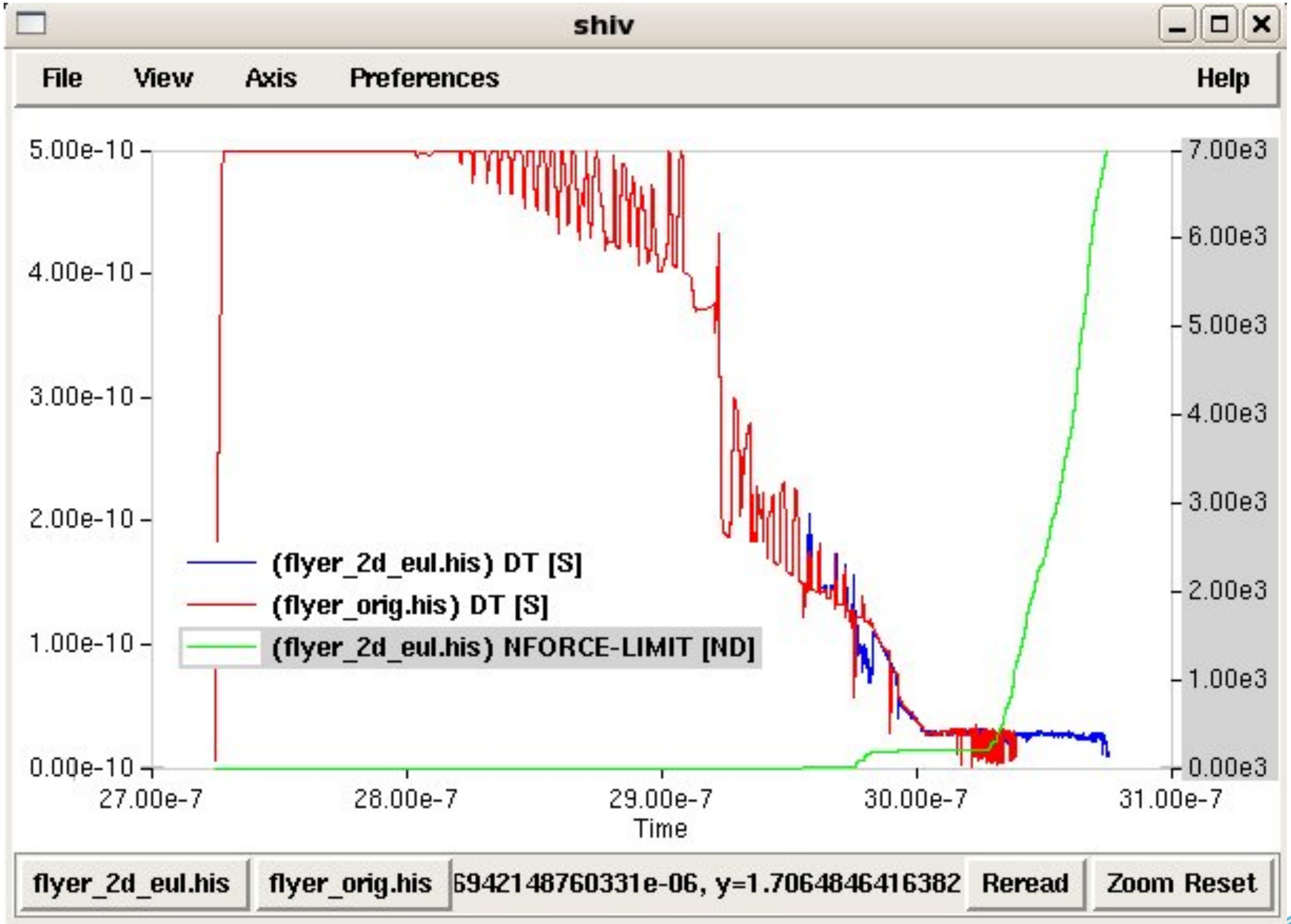
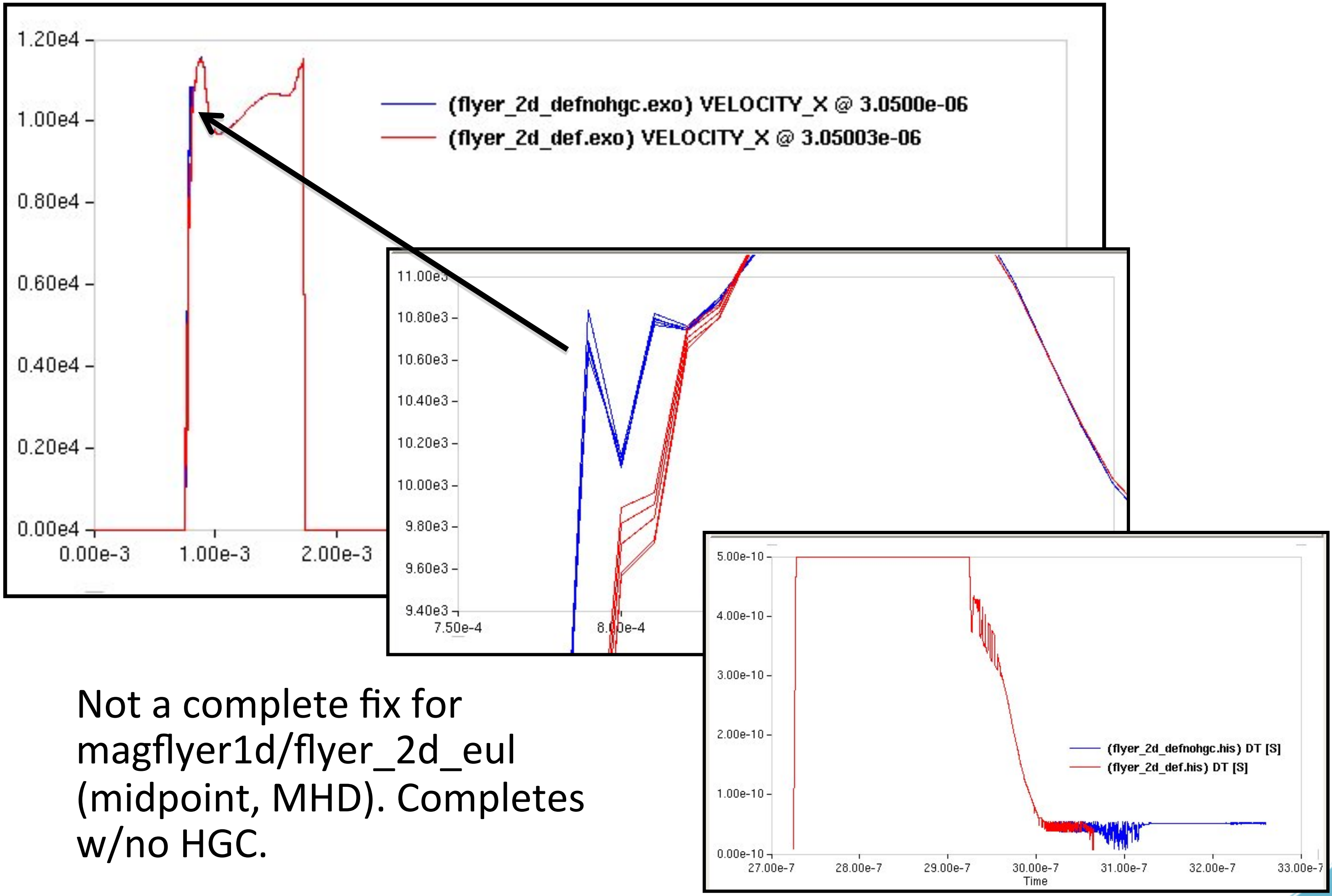
Code resilience: node max force limiter effect

- Magflyer1d (mhd, midpoint) as test



6

Code resilience: node max force limiter effect



Not a complete fix for magflyer1d/flyer_2d_eul (midpoint, MHD). Completes w/no HGC.

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6

Code resilience: modernization testing

This is an example of the sort of testing done. The regression test suite has more than 1400 tests.

Have tested two proposed new defaults, running slow/medium benchmarks with executables that have the new default incorporated:

(Counts are approximate, including some families of benchmarks):

1. Patch recovery (MHD only) [Kueny/Robinson)
   - No failures (except mhd_advect2d)
   - 11 diffs
   - 6 cases override the default
2. Midpoint time integrator [Kueny/Love]
   - 9 failures; sorting these out
   - 375 diffs
   - 12 contact algorithm and 16 legacy operator splitting incompatible because central difference is hard-coded into their assumptions.

Resilience: Modern Artificial Viscosity

- Dealt with all the fails, most could be ignored
- Two could not be ignored:
  - aneosAl: shows both the previously noted time step control issue, and a coding error where the time step cannot be small enough to achieve stability.
  - Vfblock1: shows a problem with the hyperviscosity form, and the limiter implementation at boundaries.

- Changes in the code work and should allow passage.

$$Q_{hyper} = (1-\phi)(Q-\bar{Q}) \rightarrow \phi(1-\phi)(Q-\bar{Q})$$

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Resilience: Modernization tests

Four proposed defaults being tested on fast/medium/long benchmarks:

1. Patch recovery (MHD only) [Kueny/Robinson]
   -- 0 fails, 12 diffs (+14 diffs on Long problems)
   March review: 0 fail, 11 diff
2. Midpoint time integrator [Kueny/Love]
   -- 1 undiagnosed fail, 399 diffs (Long tests underway)
   March review: 9 fail, 375 diff
3. Modern Q with midpoint [Kueny/Rider/Love]
   -- 12 undiagnosed fails; 421 diffs
   March review: incomplete
4. Debar energy advection [Kueny/Robinson]
   -- Inclusion of magnetic Debar led to many fails
   March review: 9 fail, 119 diff
   -- KE+ME Debar beneficial for many problems, but conflicts with some code (e.g., XFEM), so deployment will be postponed pending further work
5. Nodal force limiter [Kueny/Petney]
   Awaiting bug fix
   March review: 4 fail, 352 diff
6. Joule heating/ s avg schemes
   Postponed

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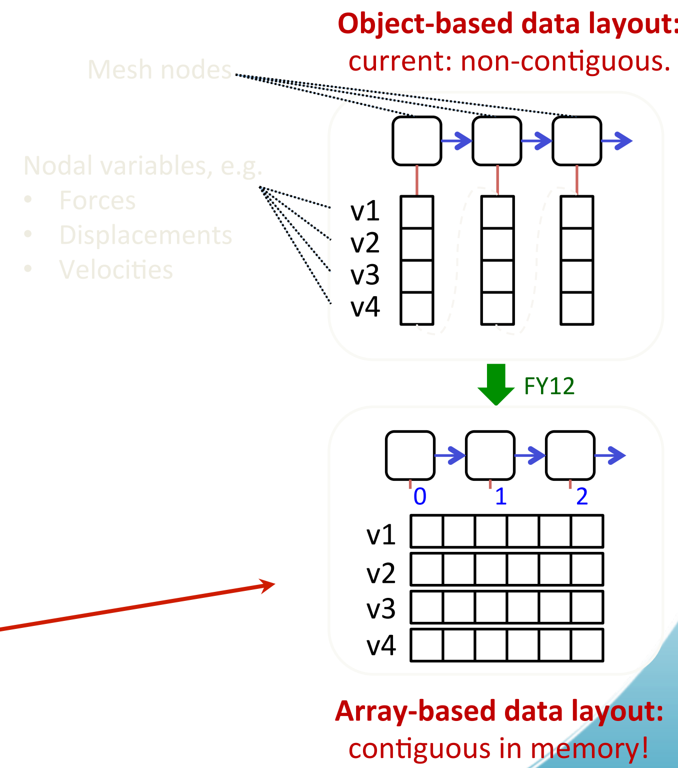
Groundwork was laid for a focused campaign toward improving speed/performance

Progression of focus from <u>robustness</u> in FY09-10 to <u>performance</u> in FY11-12 is natural, necessary, and timely.

- Consider: need for uncertainty quantification, changes in architectures.

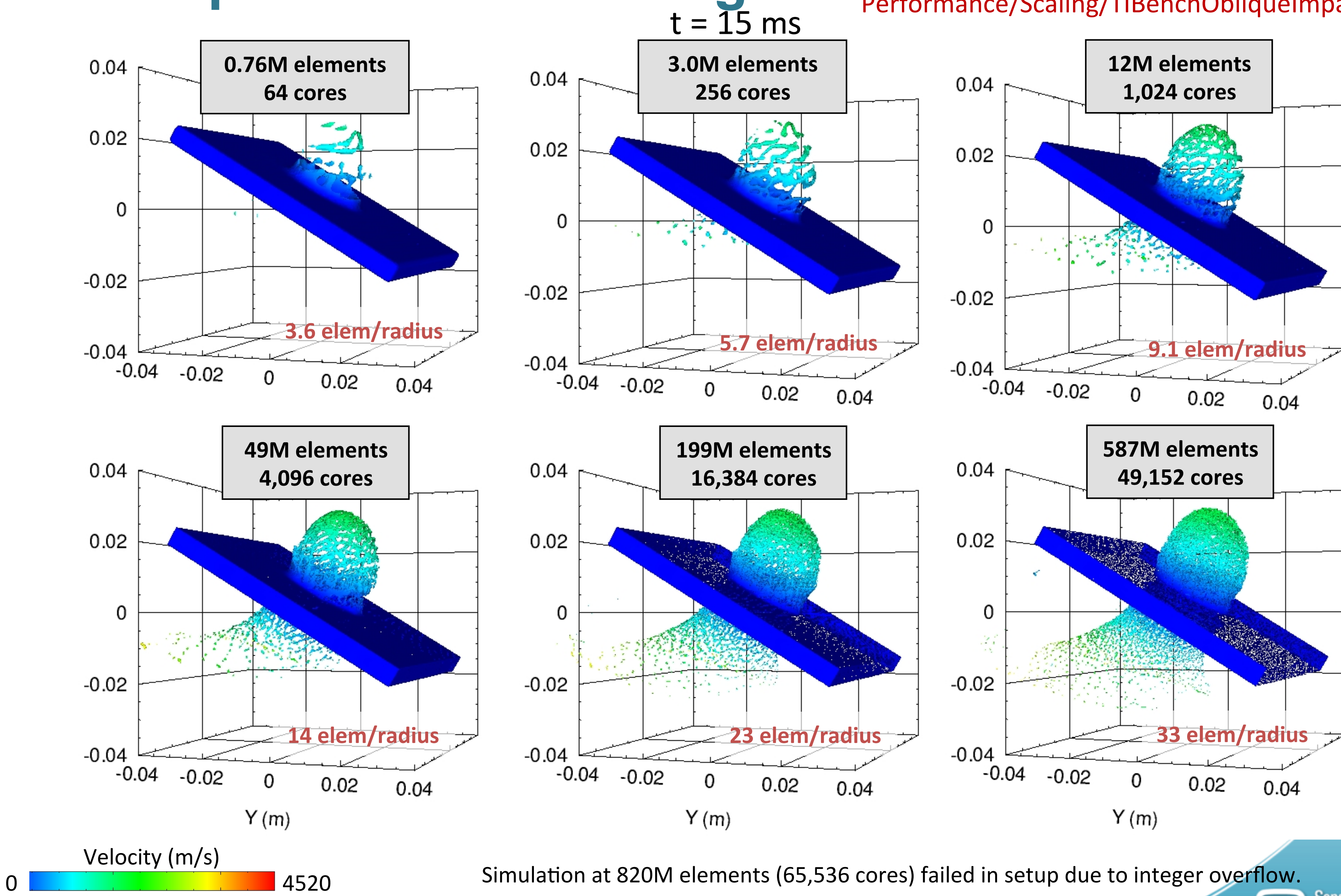
FY11: planning, scoping studies

- Platform-independent diagnostics were implemented.
- Initial quick study exposed performance hot spots, which were fixed with immediate benefit.
- Solidified FY12 strategy
  - Remap code is the most worthy target.
  - Data layout in memory offers biggest gain.
  - Easy: switch to **array-based layout**.
  - Harder: refactor code to exploit new layout.
  - Boon for running on new architectures.



Cielo performance testing

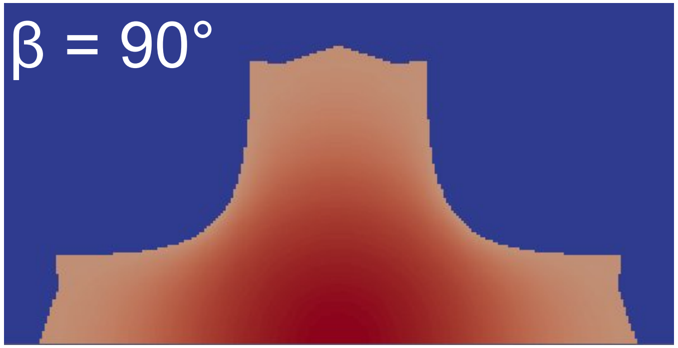
Performance/Scaling/TIBenchObliqueImpact

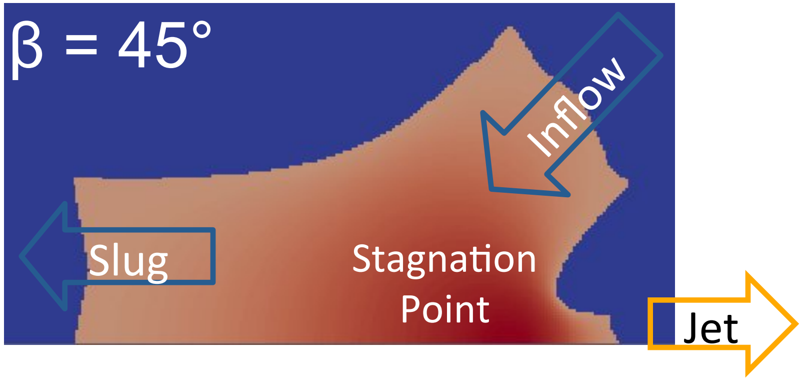


Simulation at 820M elements (65,536 cores) failed in setup due to integer overflow.

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

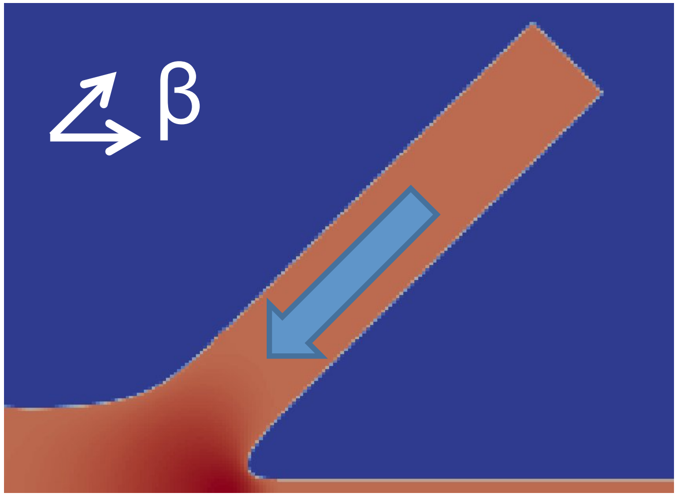
- **CJETB code exodus solutions**

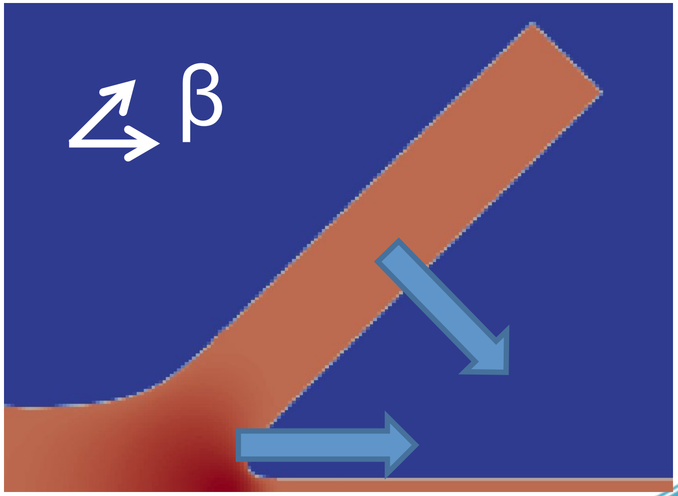




- **Simulations – 2 incident angles, 2 frames of reference**

Stagnation Point Frame of Reference

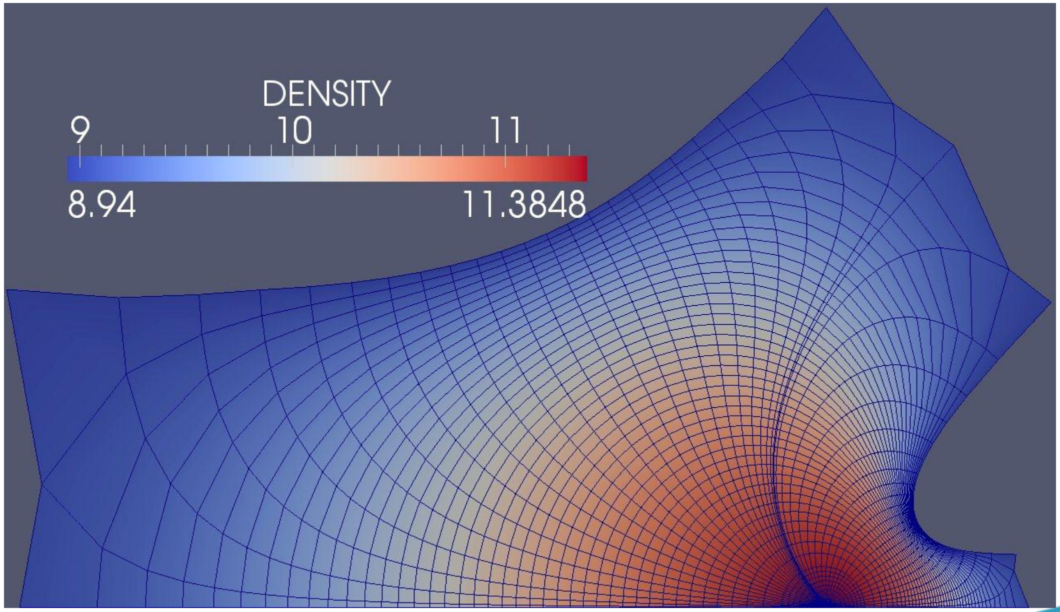




Laboratory Frame of Reference

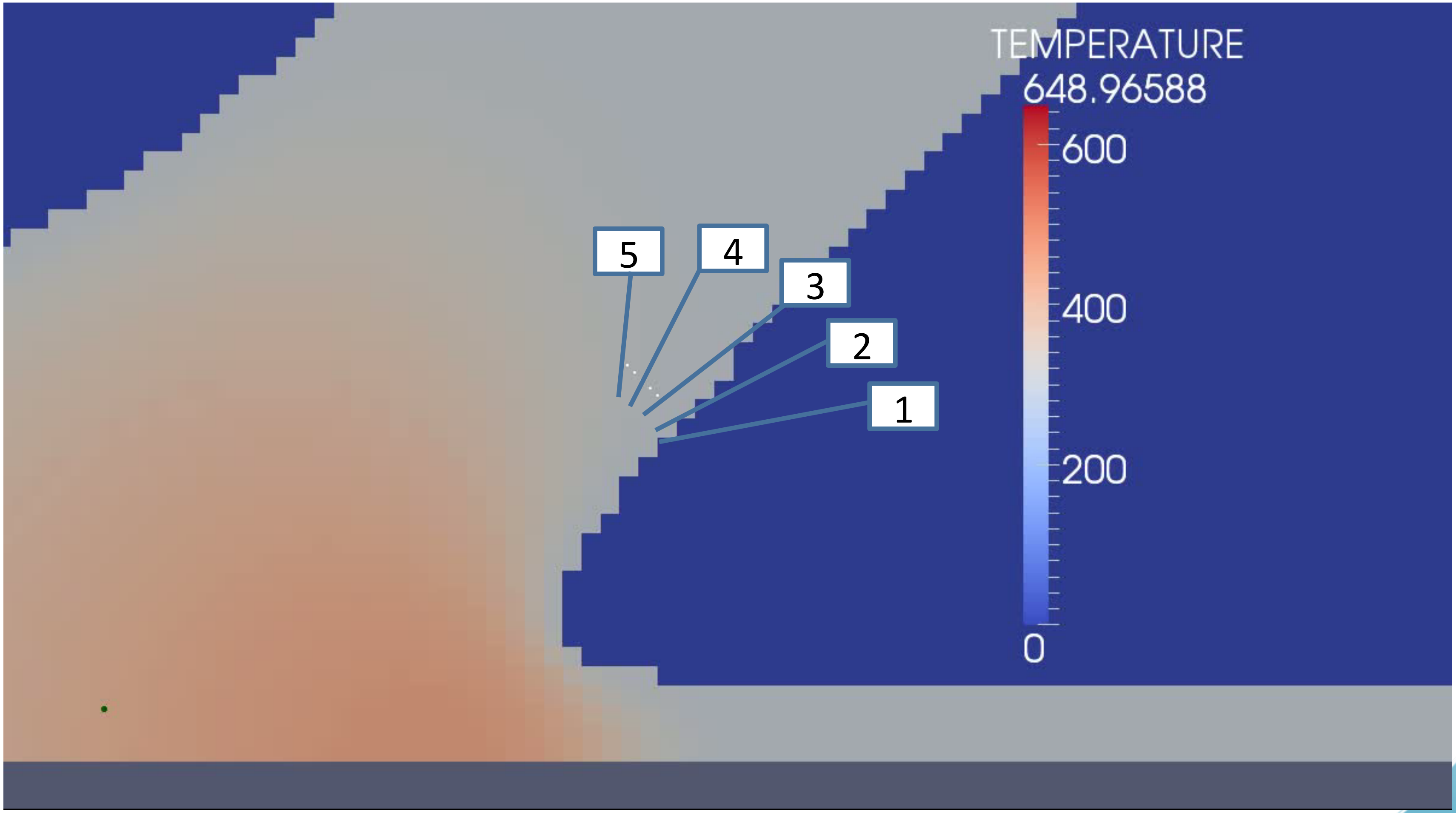
Exact Solution

- **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 and V*
- **Hanks has built a detailed permanent testing infrastructure in ALEGRA test suite.**



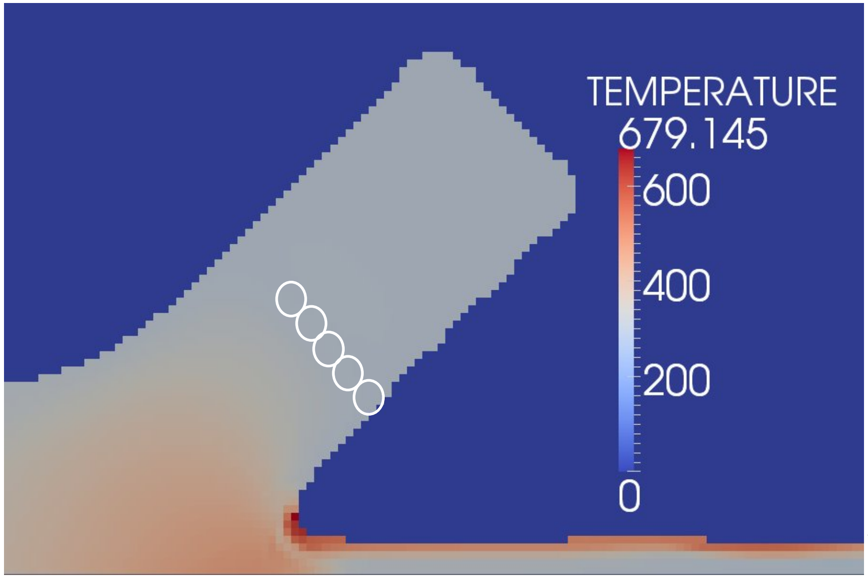
Lagrangian Tracers

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

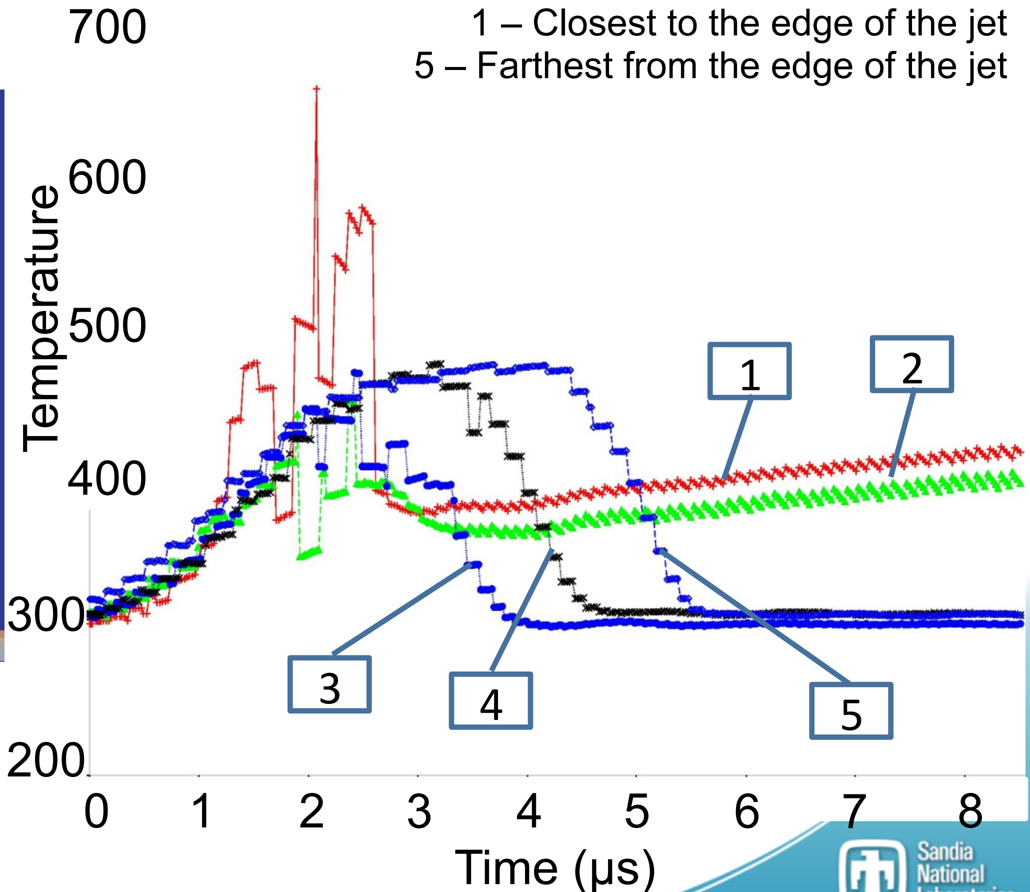


Heating Along the Jet – Under Resolved

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

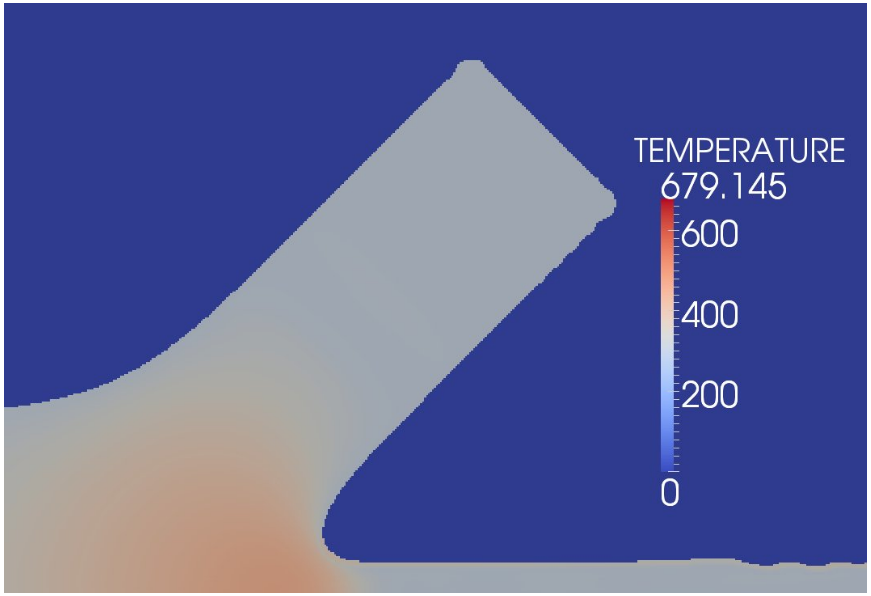


8.5 μs

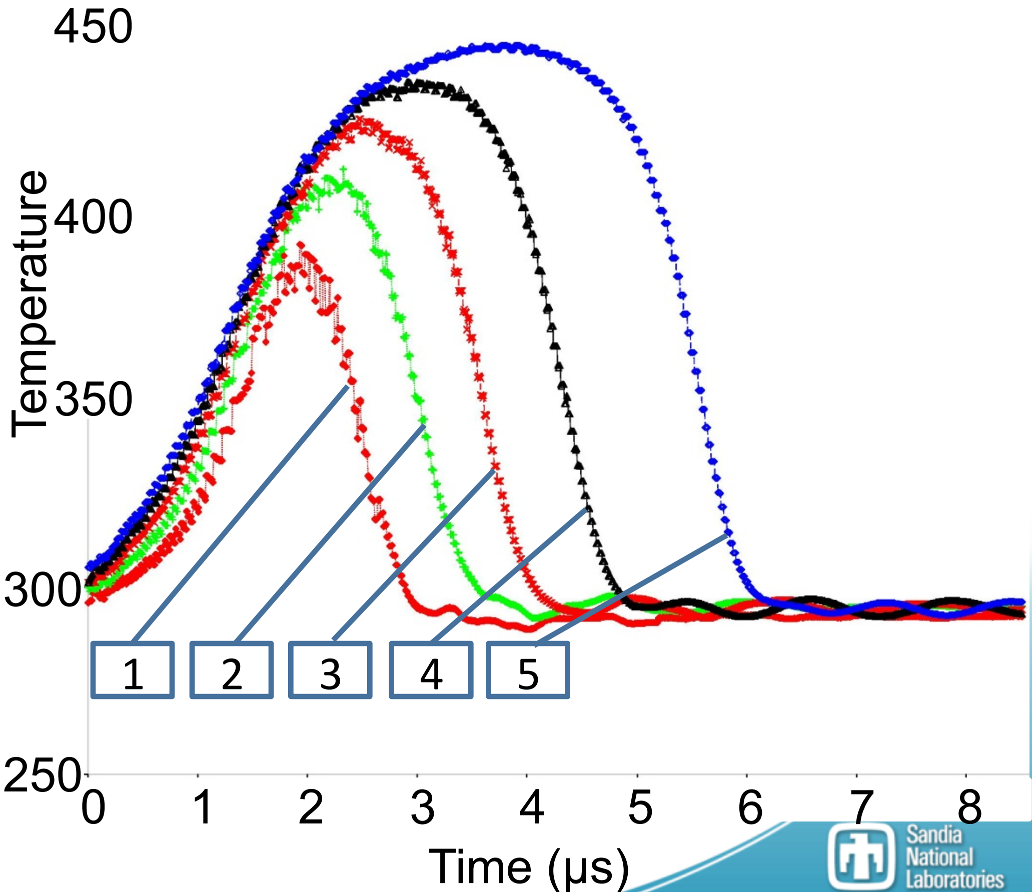


Resolution Study

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

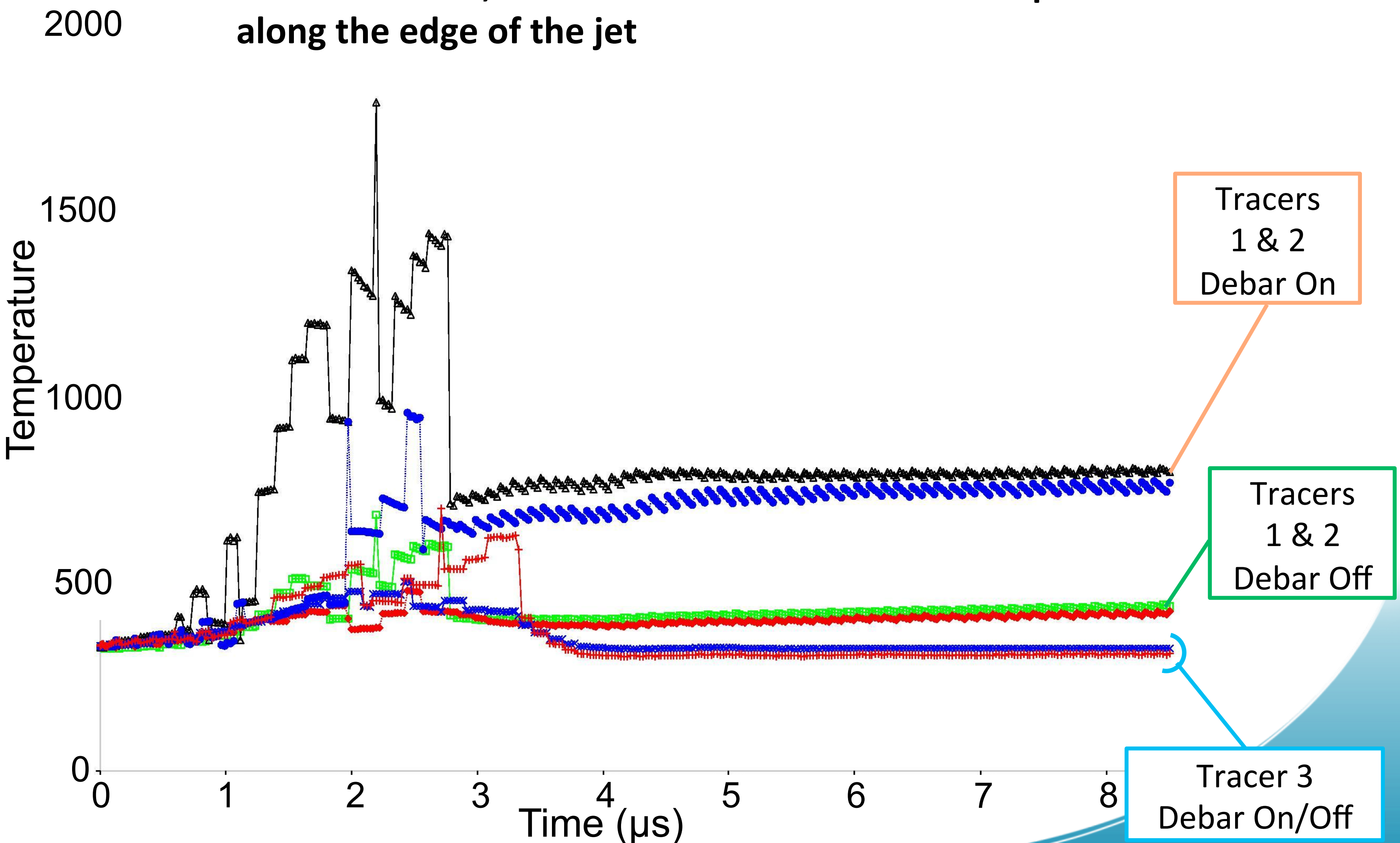


8.5 μs



Debar Energy Advection ON/OFF
Under Resolved

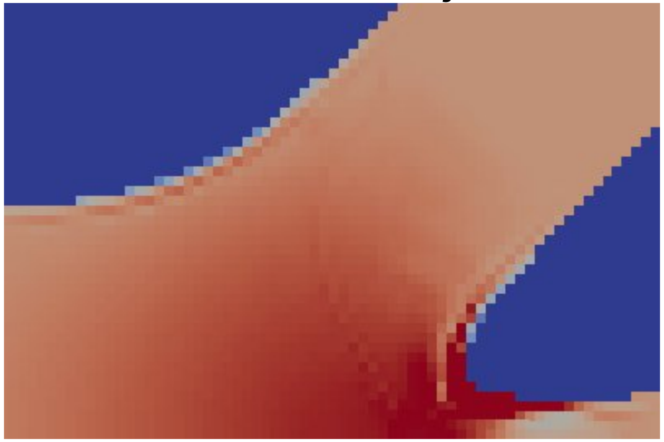
- **With Debar On, tracers 1-2 show increase in temperature along the edge of the jet**



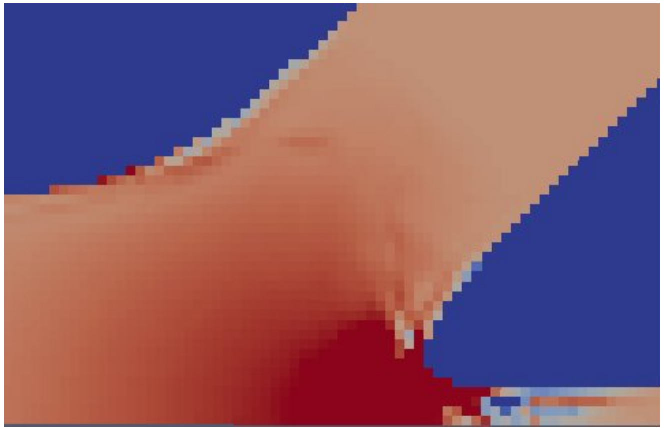
Debar Energy Advection – Resolved

- **Temperature irregularities are still seen with a resolved mesh**

4 elements across jet

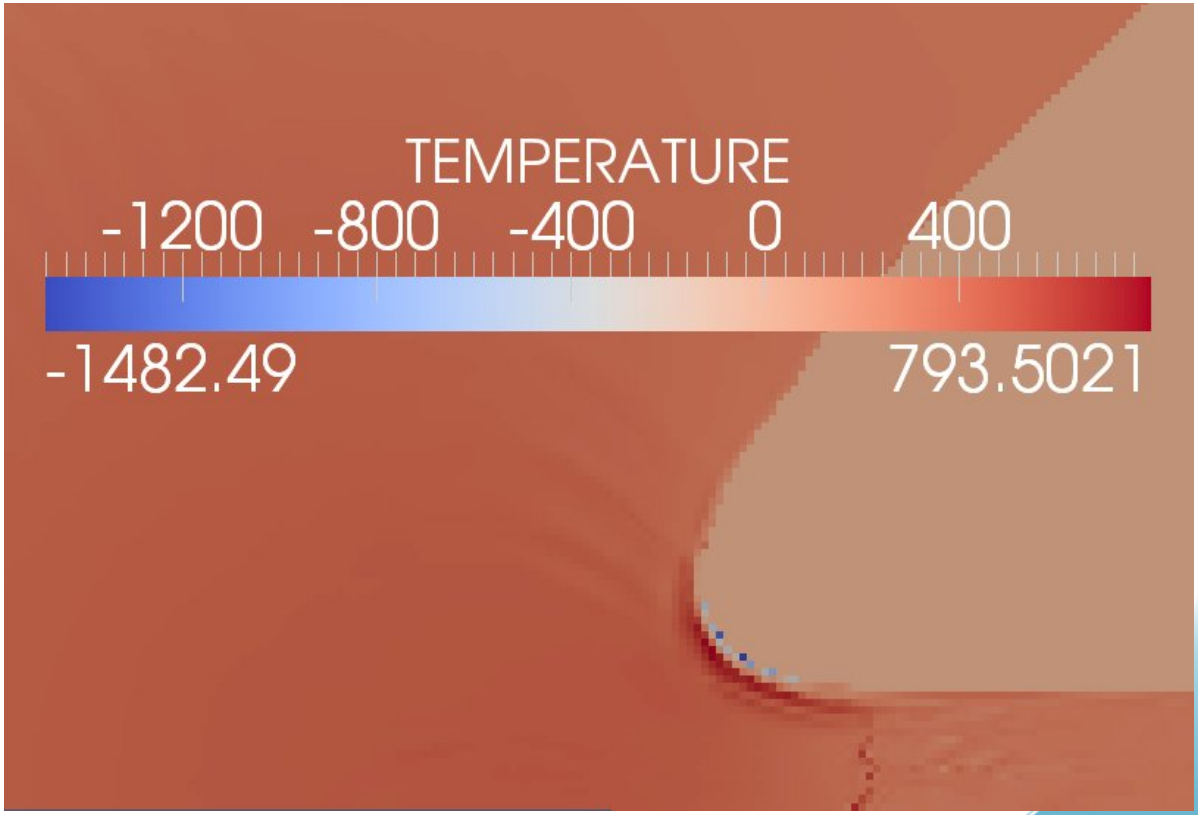


Stagnation Point Frame



Laboratory Frame

16 elements across jet



Standard Artificial Viscosity Limiter and Hyperviscosity ON/OFF

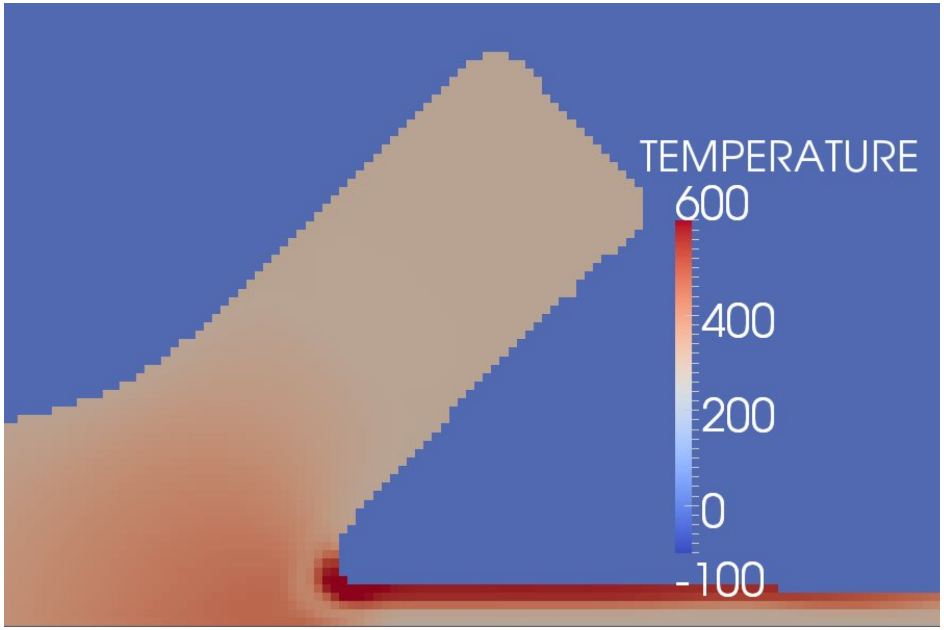
45° Lab Frame case shown below at 8.5 µs

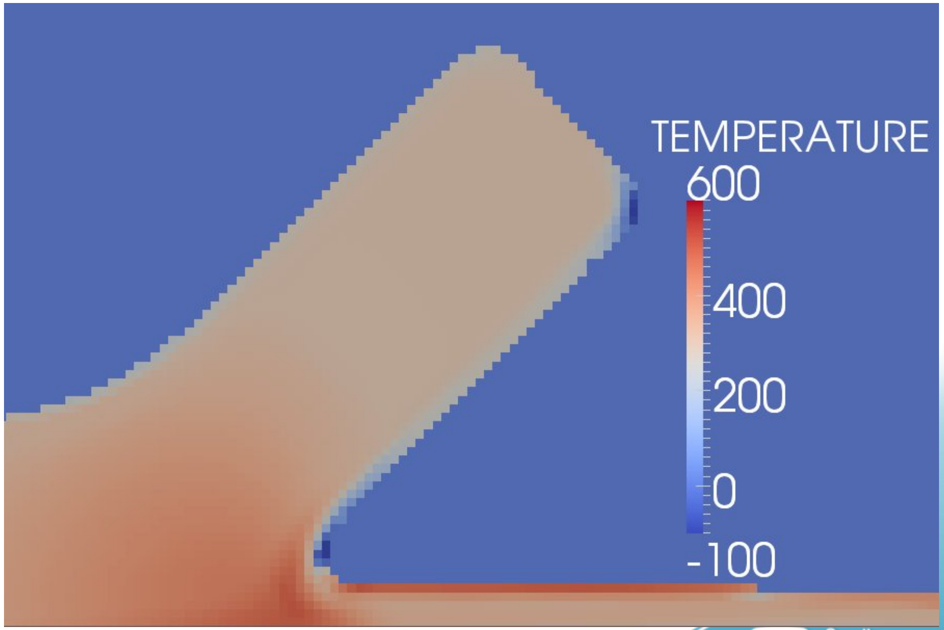
<u>Standard Artificial Viscosity – Default Settings</u>

Linear	0.15
Quadratic	2.0
Expansion Linear=	OFF
Expansion Quadratic=	OFF
Limiter =	OFF
Hyperviscosity =	0.0

<u>Standard Artificial Viscosity – New Settings</u>

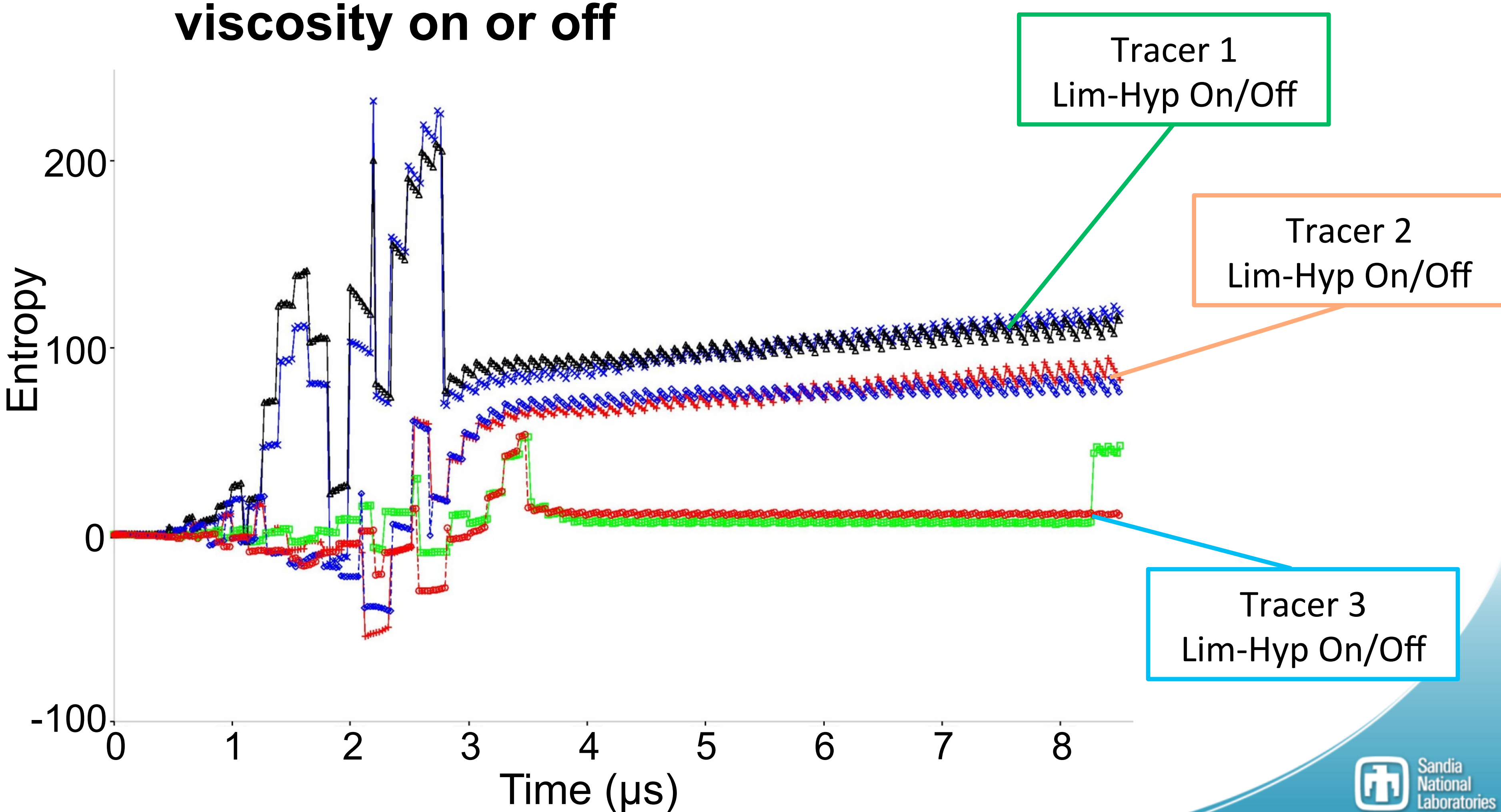
Linear	1.00
Quadratic	2.5
Expansion Linear=	ON
Expansion Quadratic=	OFF
Limiter =	ON
Hyperviscosity =	1.0





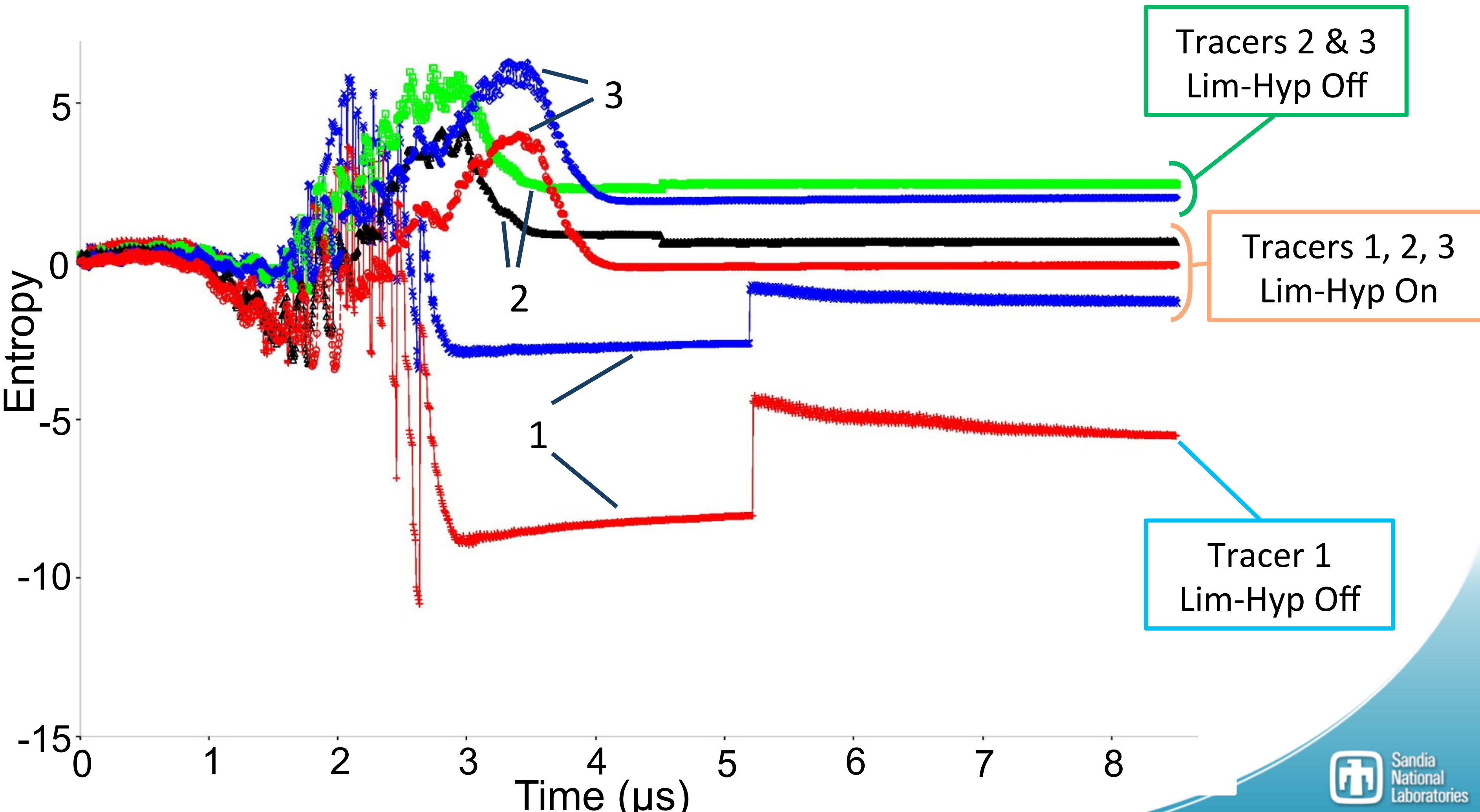
Entropy
Limiter and Hyper Viscosity ON/OFF

- **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**



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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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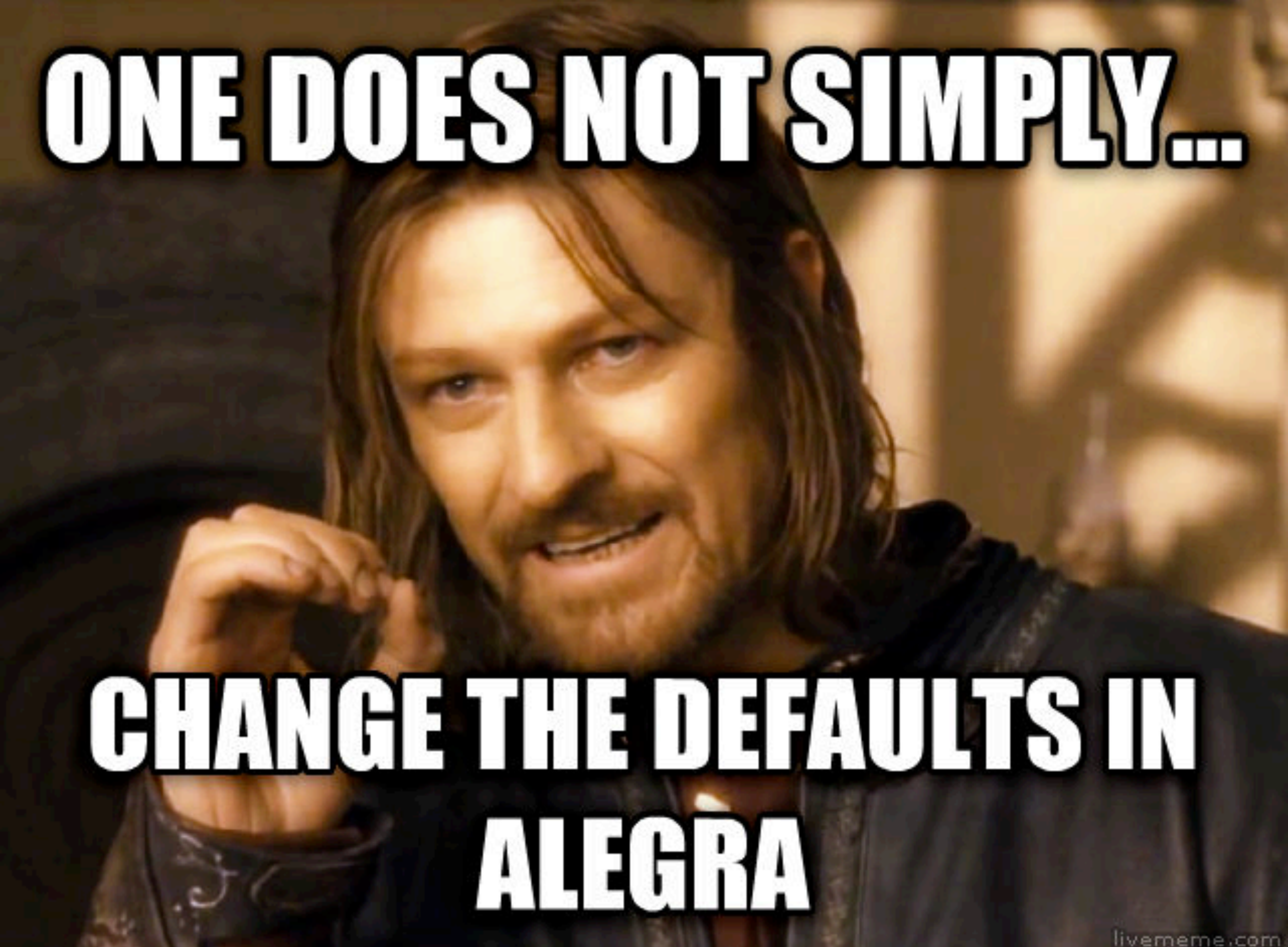
ONE DOES NOT SIMPLY...
CHANGE THE DEFAULTS IN ALEGRA
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