SAND2011-3199C

The ALEGRA Story: From Crisis to Triumph

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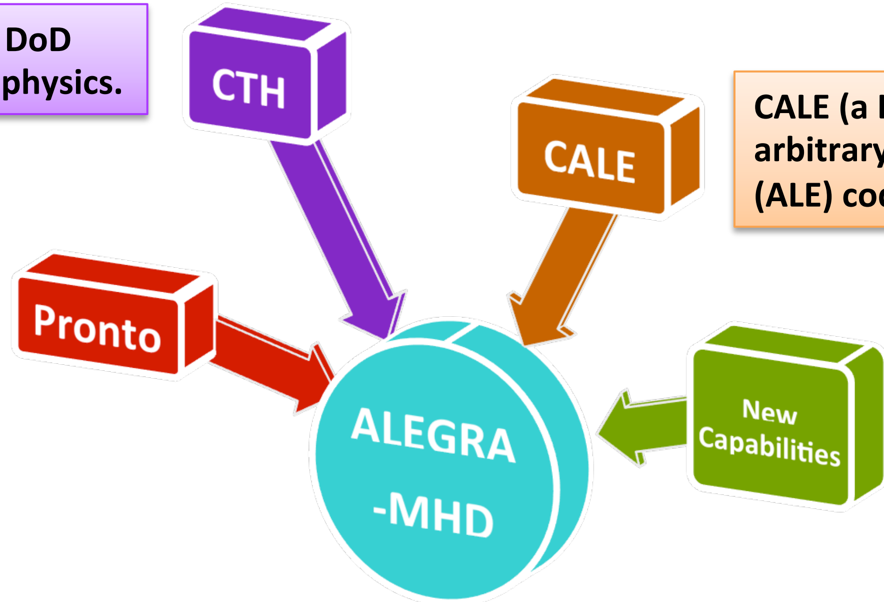
Shock and Multiphysics Department (1443)

CIS External Panel Review

May 11-13, 2011

ALEGRA is a multi-physics hydrocode developed over the last 20 years.

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



CALE (a LLNL code) 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 (DFT-MD), XFEM and railgun/coilgun simulation capability.

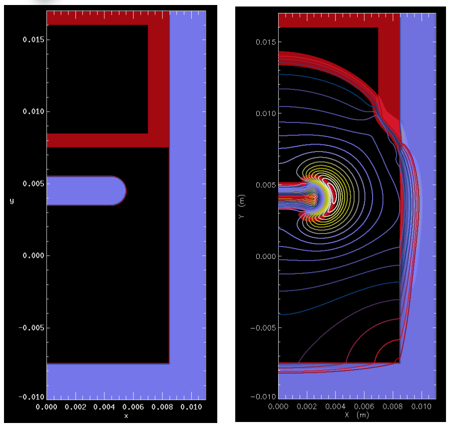
What is a "hydrocode" ?

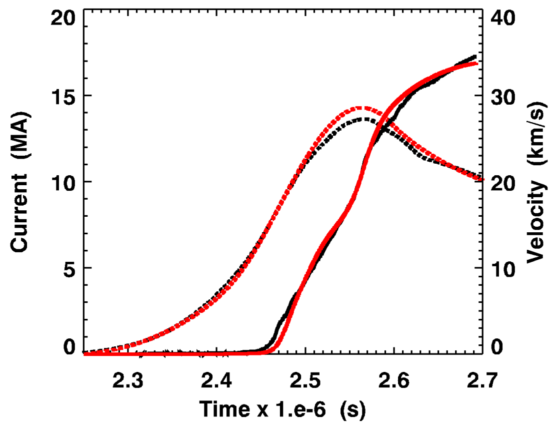
- A solution of the conservation equations using a fluid approximation including shock physics and high-strain rate material deformation.
- Uses artificial viscosity for shocks

Defining capabilities in ALEGRA

- Mimetic magneto-hydrodynamics (MHD)
- High fidelity materials
- Optimization and UQ linkage to DAKOTA
- Robust modeling of applications

In 2007 the ARL* connection was growing and our HEDP**-ASC funding was coming to an end.

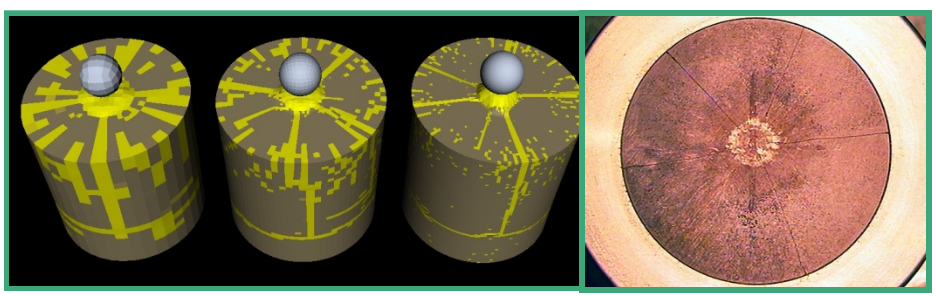




Electromagnetically driven flyer plate experimental design and analysis.

*ARL=Army Research Lab
**HEDP=High Energy Density Physics

- **At SNL ASC had decided to focus funding on SIERRA, and decrease HEDP funding. HEDP was working toward fusion as an emphasis.**
- **ARL funding had grown substantially based on unique capability for MHD and material modeling. (next slide)**



Brittle material modeling with proper physical dependence and experimental comparison. See Erik Strack's talk from this review 3 years ago for more detail.

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The lessons learned from our HEDP collaborations enabled success in modeling electro-magnetic armor.

"The advances made in ALEGRA by SNL will certainly fill the very likely modeling capability void for next generation, complex protection systems" – Mike Keele, ARL Experimental Program Lead

"MHD modeling is important to our future, and ALEGRA is the only code we have for MHD modeling" – Todd Bjerke, ARL Impact Physics Branch Chief

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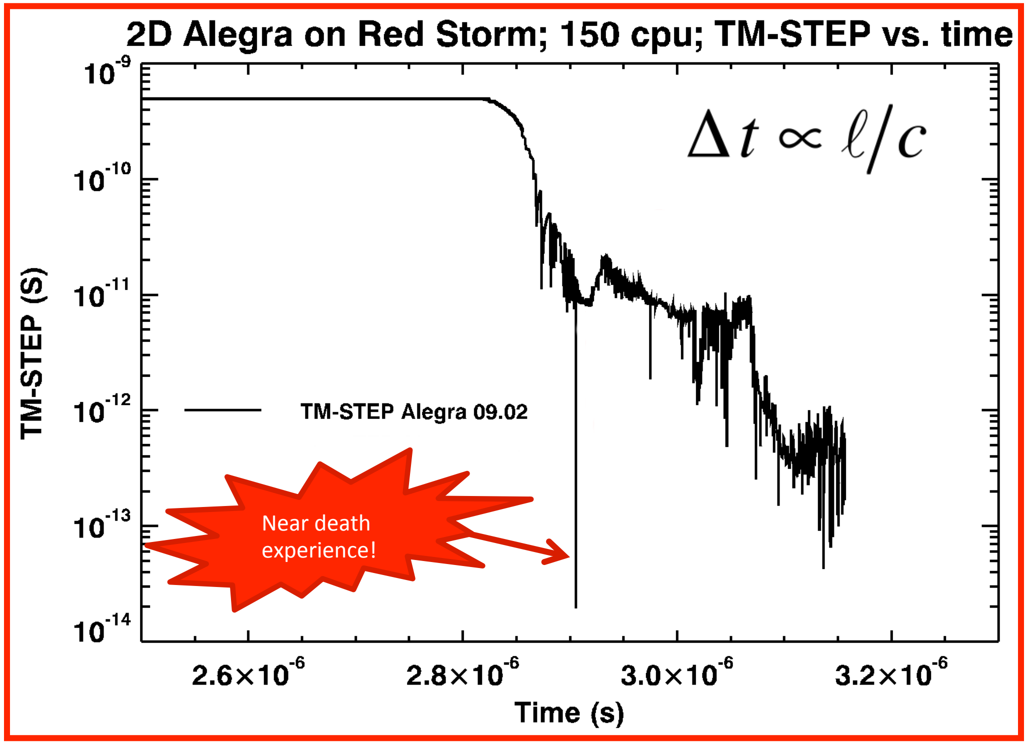
The project had grown from 2 to 8 FTEs over several years due to our success.

With our growing ARL funding there were significant issues arising due to our lack of code robustness on their applications.

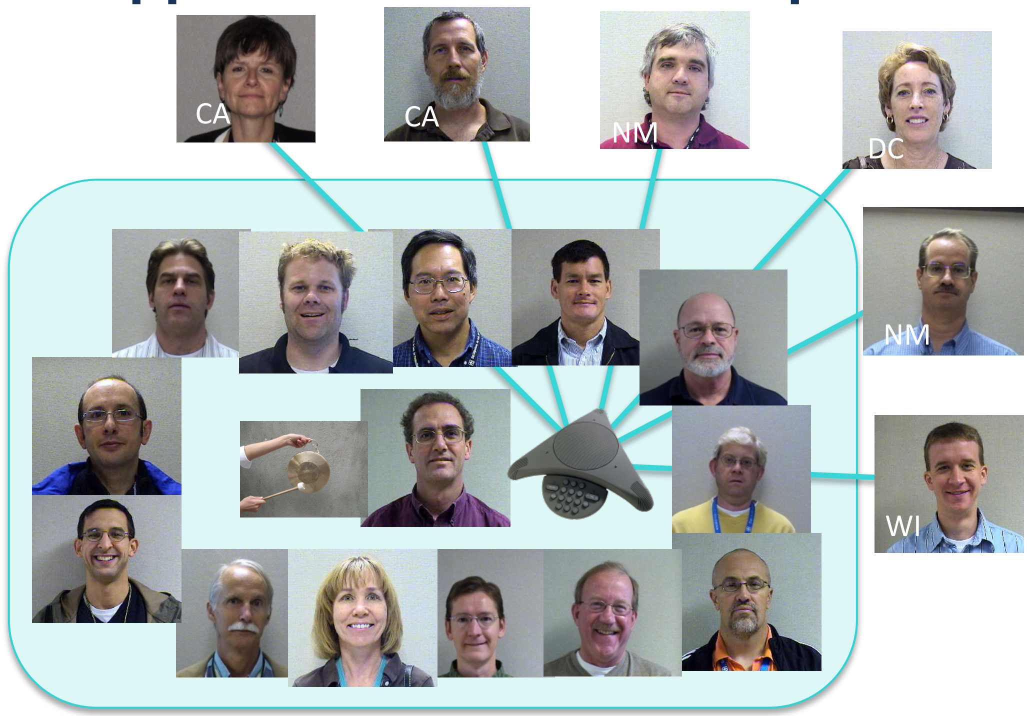
- **ARL liked what we could do, but warned us about issues.**
- **The project would wind down unless we produced a more robust code.**
- Users had grown to expect the code to run poorly or outright fail for almost any simulation of consequence
- **NONE of the important ARL application problems ran successfully to completion.**



This plot shows a typical time step trace for ALEGRA in this time period.

Part of our solution to these challenges was to take a more integrated approach to code development.

- We immediately addressed short comings in four areas:
  - **physical modeling,**
  - **numerical algorithms**,
  - code development **attitudes,**
  - code development **practices.**
- We built a tightly knit team
  - **15 minutes daily standup meeting** ,
  - fast cycle for project planning
  - Automated testing with **user prototype**, verification & performance suites to augment the regression testing we already used.



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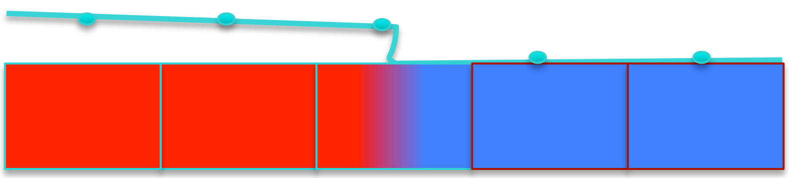
We made improvements in the remap and multimaterial methods plus the stability criteria.

Summary of remap changes*: Detect the local multimaterial flow topology



Mixed cell remap is now lower order

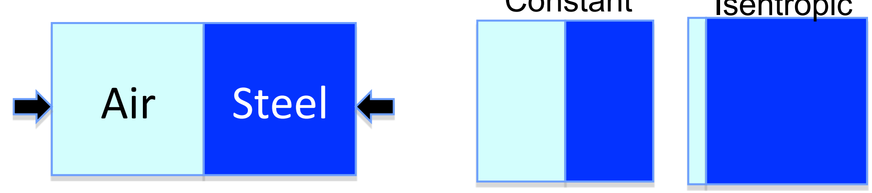
- **Alegra uses the minmod scheme (the most dissipative second order "TVD" method)**

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

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

The default pure cell remap method in ALEGRA has been changed to a compact Stencil variant of the piecewise parabolic Method (PPM, 3rd order accurate) replacing The 2nd order accurate Van Leer method.

Summary of multimaterial Lagrangian closure algorithm changes provide a physically based stable model*



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

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

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

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

*W Rider, Love, Wong, Strack, Petney, LeBreche, *Int J. Num. Meth. Fluids*, 2011
**Scovazzi, Love, Rider, *J. Comp. Phys.*, 2009.

Basic numerical algorithms have been changed for the first time since the code was founded.

Example: Improvement in the fracture model

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Old model

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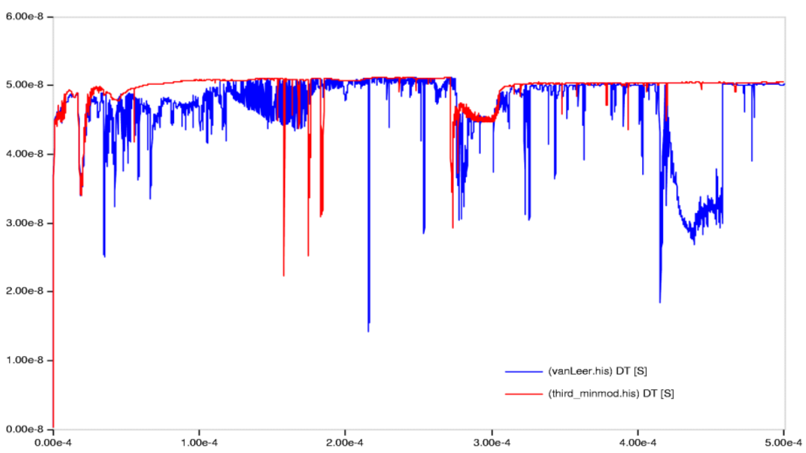
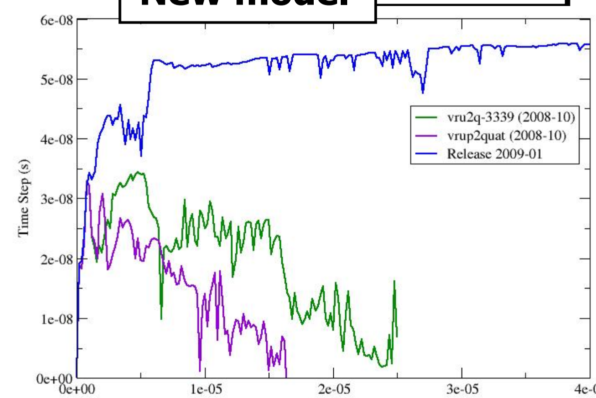
New model

Δt



The "old" time step size Traces are much better than the traces during the period when ARL warned us.

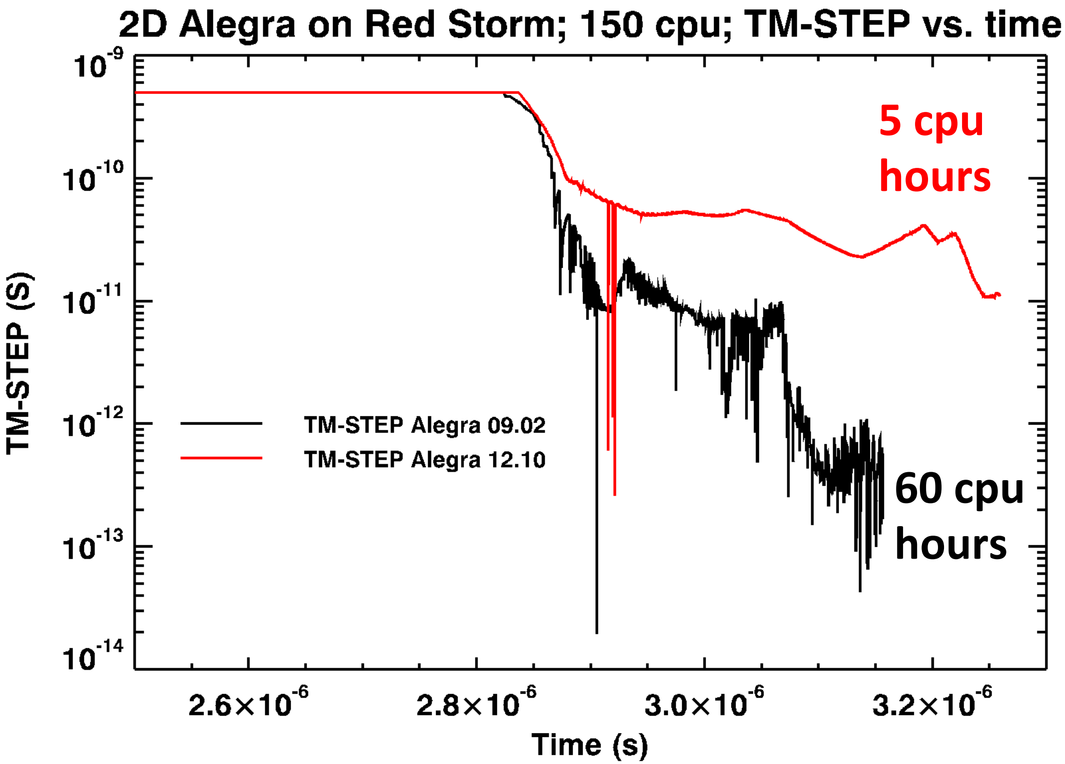
Bill Rider - CIS



Our existing HEDP user base noticed the benefits to the changes made in code robustness.

- 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 thought 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!

ALEGRA simulations enabled successful FY11 NW HEDP related experiments

Despite our progress, the future holds new challenges that will continually test our progress.

- We can never rest, we are never good enough,
  - *Our processes must continually improve*
  - *We must maintain a strong customer focus*
- **We are starting to deliver similar results for our NW mission.**
  - Electro-Mechanics modeling
  - Exploding bridge wire
  - Lightning
  - HEDP support for dynamic materials experiments.

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This year our ARL funding supports 14 FTEs.

Supplementary Information

The ALEGRA Team

- 1443 - Allen C. Robinson (PI) John Carpenter, Susan Carroll, Richard Drake, Chris Garasi,, David Hensinger, Marlin Kipp, Duane Labreche, Edward Love, Christopher Luchini, Jay Mosso, John Niederhaus, Sharon Petney, Bill Rider, Chris Seifert, O. Erik Strack, Mike Wong, Thomas Voth
- Other 1400: V. Greg Weirs, Guglielmo Scovazzi, Tim Trucano, Jim Kamm, Brian Adams, Curt Ober, Randy Summers, Pavel Bochev
- 1641/1646: Thomas Gardiner, Thomas Haill, Heath Hanshaw, Ray Lemke, Mike Desjarlais, Kyle Cochrane,Josh Robbins
- LANL: John Walter, Kristi Brislawn
- ARL: Bob Doney, Melissa Love, Frank Murphy, Ben Chamish, George Vunni, Clint Nicely, Melissa Love, Brian Leavy, Casey Uhlig,
- LLNL: Thomas A. Brunner
- Past Developers: James Peery, Kent Budge, Mark Christan, Mike McGlaun, Dan Carroll, Rebecca Brannon

Governing Equations

- Mass $$\frac{\partial f_k \rho_k}{\partial t} = -\nabla \cdot \left(f_k \rho_k \left(\mathbf{u} - \mathbf{u}_g\right)\right)$$
- Momentum $$\frac{\partial \rho \mathbf{u}}{\partial t} = -\nabla \cdot \left(\rho \left(\mathbf{u} - \mathbf{u}_g\right) \mathbf{u} - \mathbf{T} - \mathbf{T}^M + p_r \mathbf{I}\right) + \mathbf{b}$$
- Energy $$\frac{\partial \rho \left(e + e_r + 1/2\mathbf{u}^T\mathbf{u} + 1/2\mathbf{B}^T\mathbf{B}\right)}{\partial t} =$$
$$- \quad \nabla \cdot \left[\rho \left(\mathbf{u} - \mathbf{u}_g\right) \left(e + e_r + 1/2\mathbf{u}^T\mathbf{u} + 1/2\mathbf{B}^T\mathbf{B}\right)\right]$$
$$- \quad \nabla \cdot \left[\mathbf{u}\left(\mathbf{T} + p_r\right) + \left(\mathbf{u}\mathbf{B}\right)\mathbf{B} - \mathbf{q}\right] + \mathbf{u}^T\mathbf{b} + S_e$$

- Magnetics - Faraday’s law
$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \left(\mathbf{B} \times \left(\mathbf{u} - \mathbf{u}_g\right)\right) + \left(\mathbf{u} - \mathbf{u}_g\right)\left(\nabla \cdot \mathbf{B}\right) + \nabla \times \mathbf{E}' = 0$$

- Involution constraint, Ampere’s law
$$\nabla \cdot \mathbf{B} = 0 \qquad \nabla \times \mathbf{H} = \mathbf{J}$$

Governing Equations: Radiation Included

- Energy Equation $$\frac{\partial\left(\rho\epsilon + e_r + \frac{1}{2}\mathbf{u}^T\mathbf{u} + \frac{1}{2\mu_0}\mathbf{B}^T\mathbf{B}\right)}{\partial t} =$$

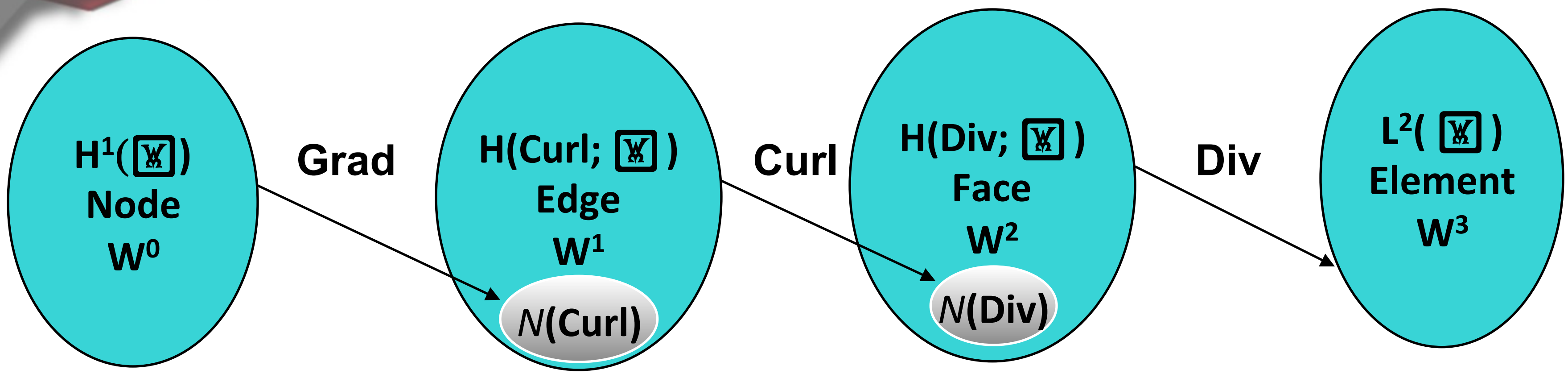
$$-\nabla\cdot\left(\rho\left(\mathbf{u}-\mathbf{u}_g\right)\left(\rho\epsilon + e_r + \frac{1}{2}\mathbf{u}^T\mathbf{u} + \frac{1}{2\mu_0}\mathbf{B}^T\mathbf{B}\right)\right)$$
$$+\nabla\cdot\left(\mathbf{u}\left(\mathbf{T}+\mathbf{T}^M - p_r\mathbf{I}\right)-\mathbf{q}\right)+\mathbf{J}\cdot\mathbf{E}'$$

- Ion-Electron Temperature

$$\rho\frac{de_e}{dt} = \mathbf{T}_e : \nabla\mathbf{u} - \nabla\cdot\mathbf{q}_e + \mathbf{J}\cdot\mathbf{E}' + \rho C_{Ve}\frac{\theta_i-\theta_e}{\tau_{ei}} - \int_0^\infty\left(\kappa\left(4\pi B_\nu - cE_\nu\right)\right)d\nu,$$
$$\rho\frac{de_i}{dt} = \mathbf{T}_i : \nabla\mathbf{u} - \nabla\cdot\mathbf{q}_i + \rho C_{Ve}\frac{\theta_e-\theta_i}{\tau_{ei}}$$

- Rad. $$\frac{1}{c}\frac{\partial I}{\partial t} + \mathbf{\Omega}\cdot\nabla we = -\sigma_t we + \frac{\sigma_s}{4\pi}\int_{4\pi} we\,\mathbf{\Omega}' + \sigma_a\frac{cB(T_m)}{4\pi} + S_I$$

Magneto-hydrodynamic treatment*



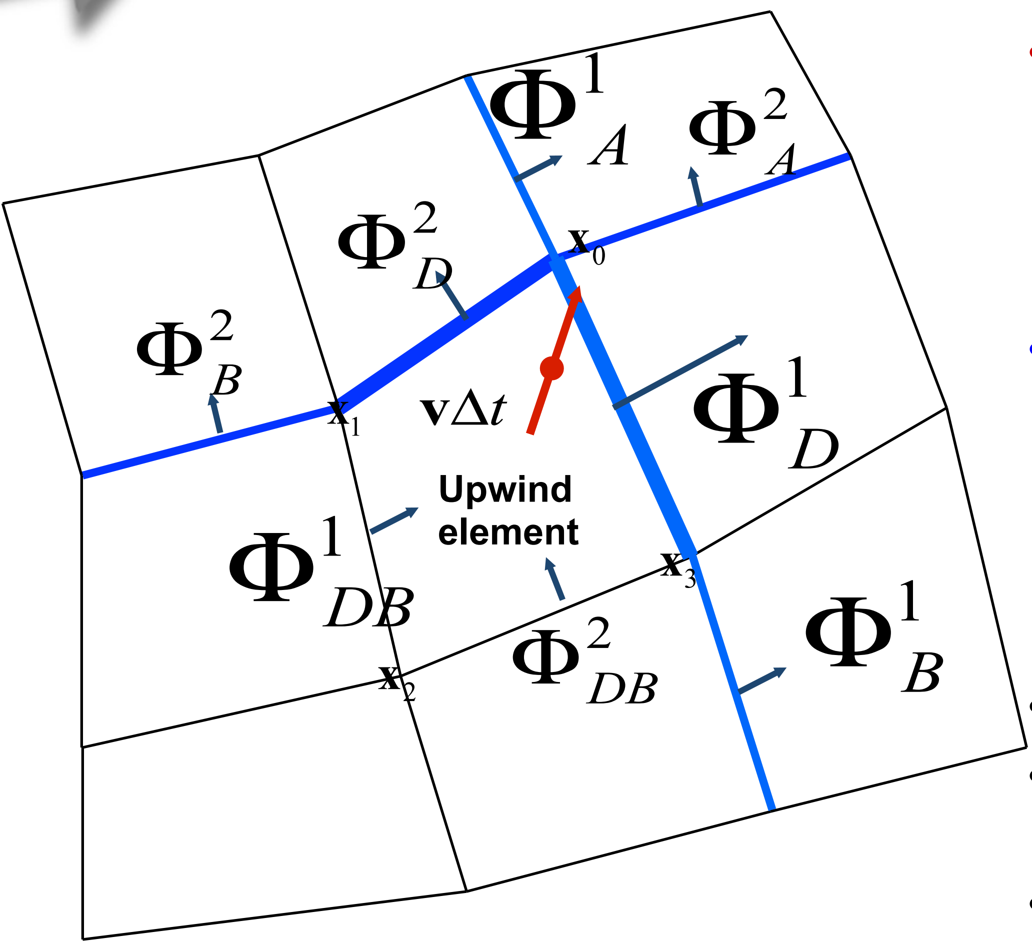
- Uses a compatible formulation that preserves the divergence free magnetic field automatically.
- A software package, *Intrepid*, makes the implementation relatively seamless with ALEGRA (and other codes)
- These properties are maintained through the remap as well.
- ALEGRA includes magnetic diffusion (using multilevel solves via Trilinos) as well as ideal MHD

*** work by Bochev and Robinson**

Magnetic Flux Density Remap

- The Lagrangian step maintains the discrete divergence free property via flux density updates given only in term of curls of edge centered variables.
  - The remap should not destroy this property.
- Constrained transport (CT) is the name for a basic approach for updating the fluxes to preserve the divergence free property.
  - CT is fundamentally unsplit.

CT on unstructured quad and hex grids (CCT)



- Define the low order or donor method by integrating the total flux through the upwind characteristic of the total face element representation of the flux density.
- High order method constructs a modification to the flux so that it varies across the element face. Compute flux density gradients in the tangential direction using the blue and the green faces.
- All contributions are combined.
- Electric field updates are located on edges.
- Take curl to get updated fluxes.
- *Requires tracking flux and circulation sign conventions*.

Montage of applications for Validation

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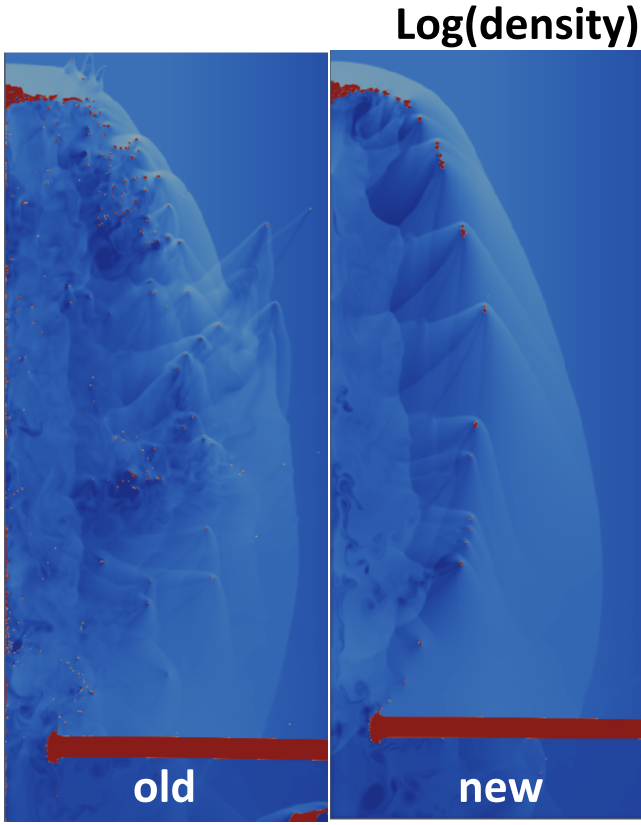
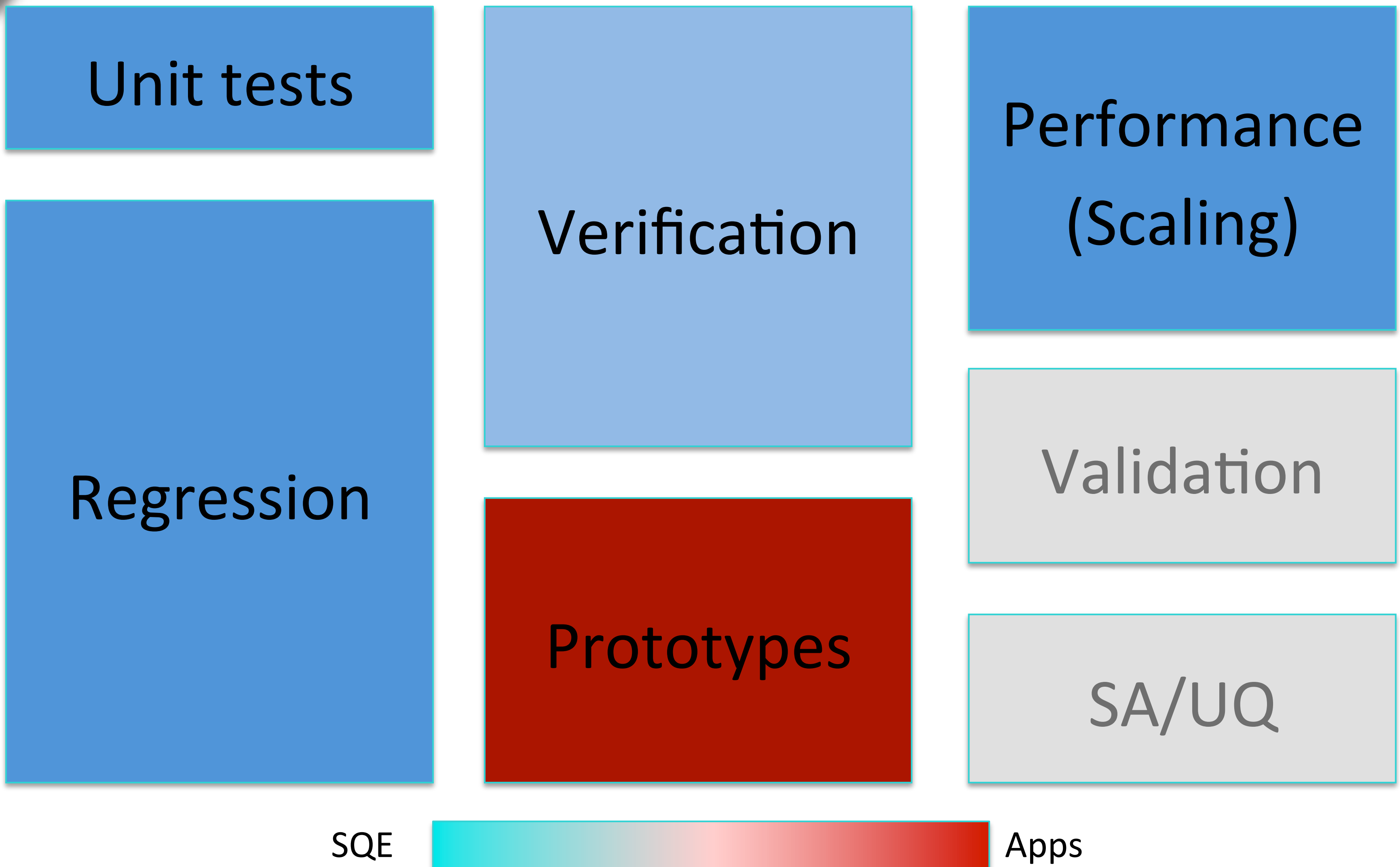


- Whipple – a classical satellite shield impact

Our team and software process



Publications 2010-2011

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Leavy, R Brian, Rebecca M Brannon, O Erik Strack, "The Use of Sphere Indentation Experiments to Characterize Ceramic Damage Models," *Journal Article,* International Journal of Applied Ceramic Technology, Submitted June 2010.

Kamm, James R., Mikhail J. Shashkov, William J. Rider,"A new pressure relaxation closure model for one-dimensional two-material Lagrangian hydrodynamics," *Journal Article,* European Physics Journal Web of Conferences, Vol. 10, Article No. 00038, Accepted/Published January 2011.

Weirs, V. Gregory, "Visualizing Material Model Data Using PRISM," *Presentation,* 4th Workshop on Ramp Compression, January 2011.

Love, E., W. J. Rider, G. Scovazzi, "Artificial Viscosity Flux Limiting in Lagrangian Shock Hydrodynamic Finite Element Computations ," *Abstract,* usnccm-2011, Minneapolis, MN, July 2011.

Rider, William J, Ed Love, Gugliemo Scovazzi, "Limited Artificial Viscosity and Hyperviscosity Based on a Mollified Nonlinear Hybridization Method," *Abstract,* Multimat 2011, September 2011.

Kamm, James R., Mikhail J. Shashkov, William J. Rider, "A New Pressure Relaxation Closure Model for Two-Material Lagrangian Hydrodynamics," *Presentation,* New Models and Hydrocodes for Shock Wave Processes in Condensed Matter, 24-28 May 2010, Paris, France, May 2010.

Kamm, James R., Mikhail J. Shashkov, Jimmy Fung, Alan K. Harrison, Thomas R. Canfield "A comparative study of various pressure relaxation closure models for one-dimensional two-material Lagrangian hydrodynamics," *Journal Article,* International Journal for Numerical Methods in Fluids, Accepted/Published May 2010.

Weirs, V. Gregory, Laura P. Swiler, James R. Kamm, Marco Ratto, Stefano Tarantola, Brian M. Adams, William J. Rider, Michael S. Eldred, "A Sensitivity Analysis of the Gas Dynamics Equations," *Presentation,* XII International Workshop on Supercomputing and Mathematical Modeling, October 2010. **Weirs, V. Gregory, James R. Kamm, Laura P. Swiler, Stefano Tarantola, Marco Ratto, Brian M. Adams, William J. Rider, Michael S. Eldred,** "Sensitivity Analysis Techniques Applied to a Model Shock Problem," *Presentation,* Nuclear Explosives Code Developers Conference 2010, October 2010. **Weirs, V. Gregory, Laura P. Swiler, Marco Ratto, Stefano Tarantola, Brian M. Adams, James R. Kamm, William J. Rider, Michael S. Eldred,** "Sensitivity Analysis Techniques Applied to a System of Hyperbolic Conservation Laws, Part II," *Presentation,* Sixth International Conference on Sensitivity Analysis of Model Output, July 2010.

Weirs, V. Gregory, James R. Kamm, Laura P. Swiler, Stefano Tarantola, Marco Ratto, Brian M. Adams, William J. Rider, Michael S. Eldred, "Sensitivity Analysis Techniques Applied to a Model Shock Problem (U)," *Conference Paper,* Nuclear Explosives Code Developers Conference 2010, December 2010. **Weirs, V.Gregory, Laura P. Swiler, Marco Ratto, Stefano Tarantola, Brian M. Adams, James R. Kamm, William J. Rider, Michael S. Eldred,** "Sensitivity Analysis Techniques Applied to a System of Hyperbolic Conservation Laws, Part I," *Presentation,* Sixth International Conference on Sensitivity Analysis of Model Output, July 2010.

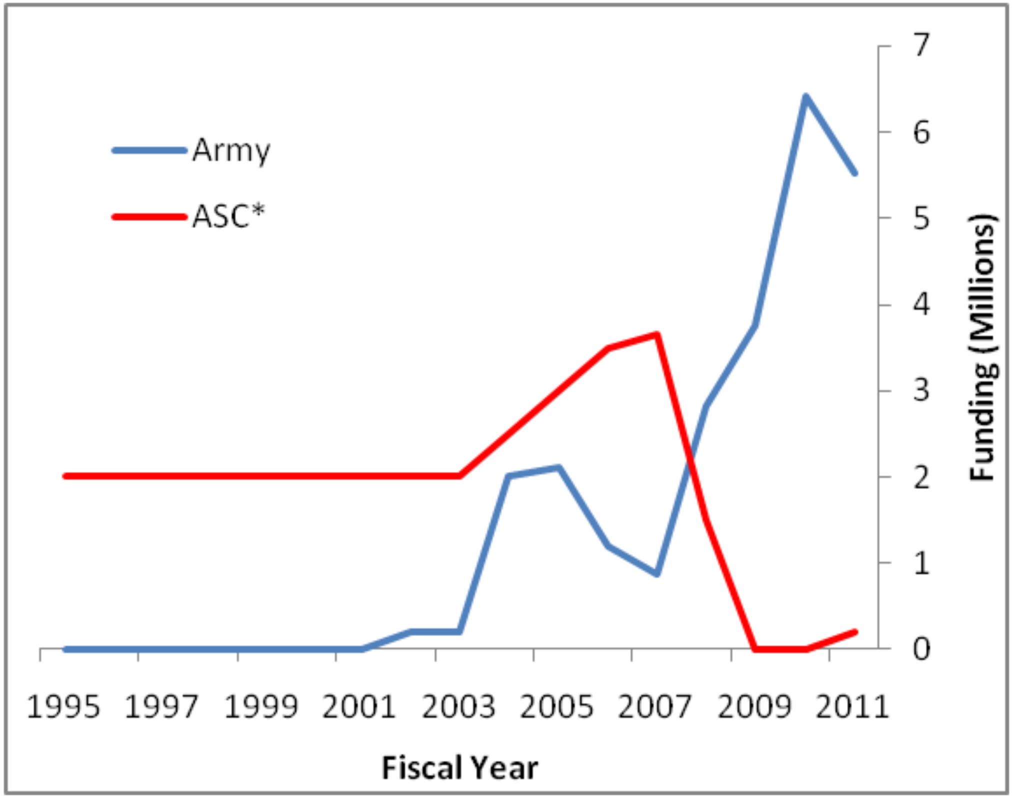
Rider, William J, "Introduction to Computational Fluid Dynamics and Verification & Validation ," *Presentation,* Modeling Experiment and Validation Summer School, July 2010.

Rider, William J, "A Rogue's Gallery to V&V in Practice," *Presentation,* MeV Summer School Lunch Talk, July 2010.

LDRD Projects Contributing to ALEGRA's development

- Electromagnetic Launch Science and Technology, PI : Garasi
- Highly Scalable Linear Solvers for Large Science Simulations on Thousands of Processors, PI: Hu
- Efficient Implicit Multigroup Radiation Calculations, PI: Brunner
- Electrical Conductivity of Metal Alloys, PI: Desjarlais
- Assessment of Advanced Pulsed Power Fusion Concepts, PI: Mehlhorn
- Advanced Fusion Concepts: Neutrons for Testing and Energy, PI: Sinars
- Thermo-Physical Properties of Shocked Water for Modeling Pulsed Power Switches and Other HEDP Systems, PI: Mattsson
- Development of Simulation and Validation Techniques for the Dynamic Behavior of Metals at the Grain Scale, PI: Vogler
- Modeling Signals from Earth-Penetrating Nuclear Weapons for Remote-Kill Assessment, PI: Dreike
- Multilevel Techniques for Unstructured Grids on Massively Parallel Computers, PI: Tuminaro

ALEGRA Funding History++



*ASC funding is approximate (except FY 2007)

++Funding does not include research foundation (CSRF), LDRD, or other