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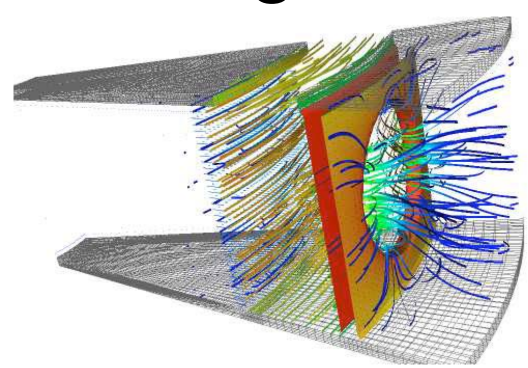
ALEGRA: An Arbitrary Lagrangian-Eulerian Multimaterial, Multiphysics Code

The ALEGRA Team

presented by Bill Rider

Sandia National Laboratories

AIAA Aerospace Science Meeting, Reno NV January 8, 2008



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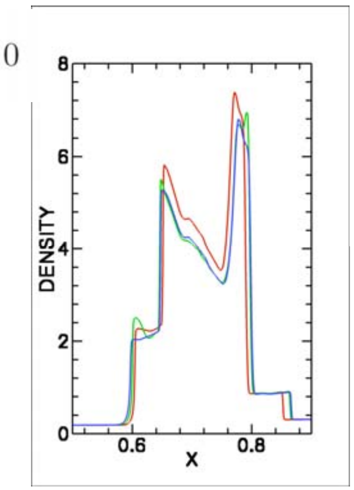
A quote to start us off

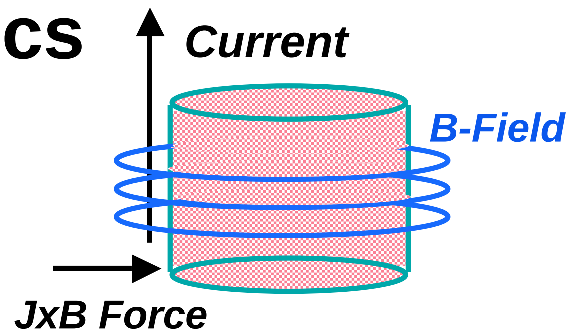
"An expert is someone who knows some of the worst mistakes that can be made in his subject, and how to avoid them."

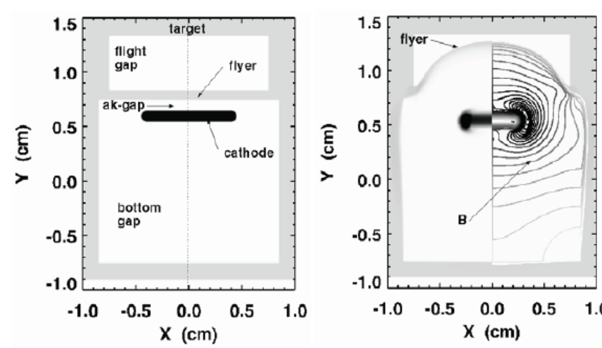
– Werner Heisenberg

Outline of the Talk

- A Brief history of ALEGRA
- Governing Equations $\frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\mathbf{B} \times \mathbf{u}) + \mathbf{u}(\nabla \cdot \mathbf{B}) = 0$
- Solution Procedure
- Multimaterial dynamics
  - Lagrangian step
  - Remap step
- MHD
- Applications
  - Code Verification
  - Z-pinch implosions
  - Advanced material modeling







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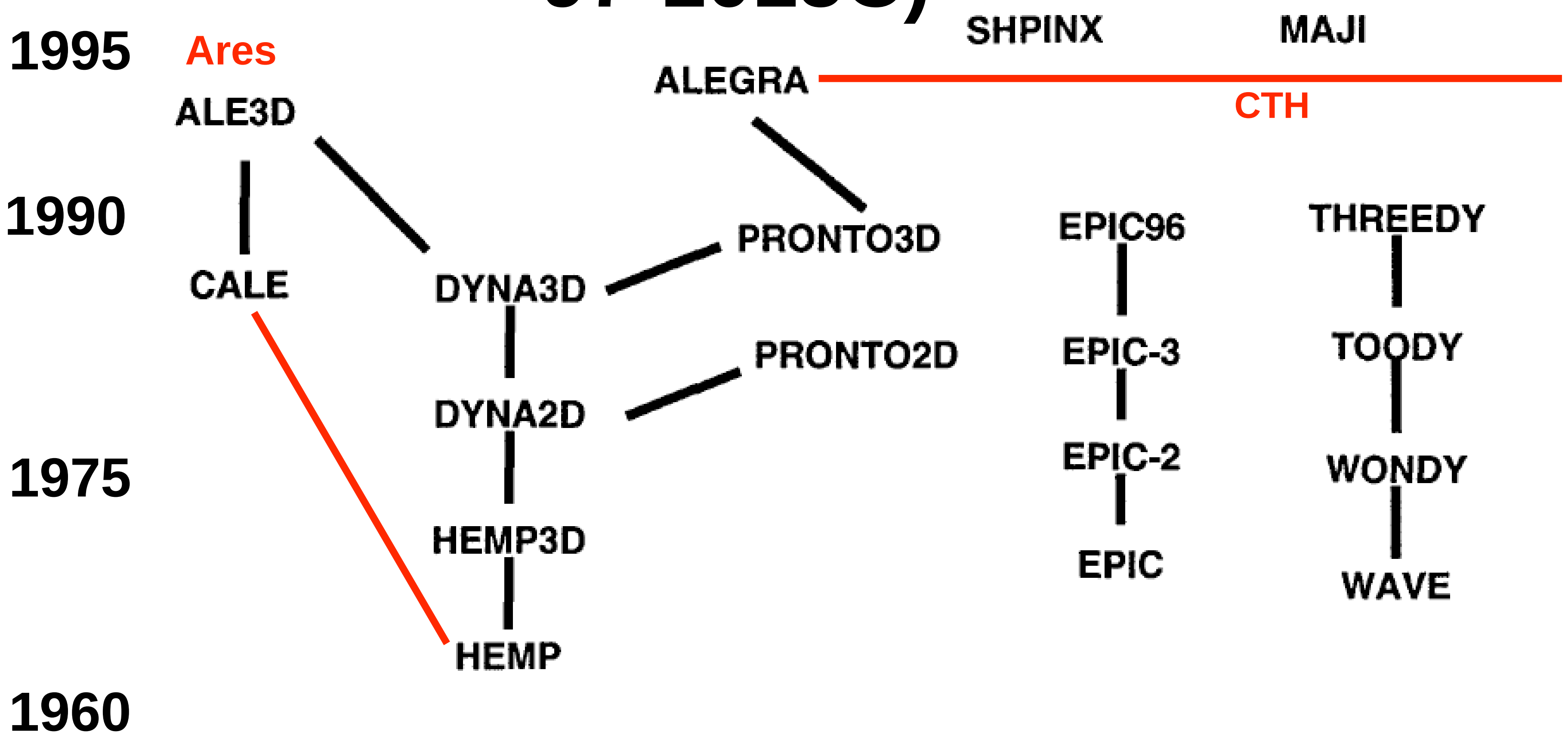
A (very) brief history of ALEGA

- The project began in 1988 to support the ICF program,
- Based on existing codes PRONTO & MMALE
- Major support and development under the DOE ASC program through the 1990's to today
- Developed in C++ for hig-performance massively parallel computers

Historical Context

- **PRONTO is the basis (became PRESTO under ASC Sierra framework)**
  - **The basic Lagrangian step is PRONTO plus the energy equation necessary for shocks (ala CTH!).**
- **It's a finite element code (we're Sandia after all!).**
- **Other aspects of the method (i.e. the ALE remap) are based on (inspired by) CTH.**

Family tree of Lagrangian hydrocodes by Gene Hertel (SAND 97-1015C)



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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**

$$\begin{aligned} \frac{\partial \rho \left(e + e_r + 1/2\mathbf{u}^T\mathbf{u} + 1/2\mathbf{B}^T\mathbf{B}\right)}{\partial t} &= \\ &- \nabla \cdot \left[\rho \left(\mathbf{u} - \mathbf{u}_g\right) \left(e + e_r + 1/2\mathbf{u}^T\mathbf{u} + 1/2\mathbf{B}^T\mathbf{B}\right)\right] \\ &- \nabla \cdot \left[\mathbf{u} \left(\mathbf{T} + p_r\right) + \left(\mathbf{u}\mathbf{B}\right)\mathbf{B} - \mathbf{q}\right] + \mathbf{u}^T\mathbf{b} + S_e \end{aligned}$$

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

Solution Procedure

- ALEGRA uses operator splitting, the key is a Lagrangian-Remap sequence for the ALE

1. Lagrangian - MHD
2. Diffusion: Magnetic-Thermal
3. Remesh
4. Remap
5. Radiation

– Repeat

Review of the two step method for (DOE) ALE codes.

1. Compute the solution to the equations in the *Lagrangian* frame (including *Q's & hourglass* control)

$$\frac{d\vec{x}}{dt} = \vec{u}; \rho = \frac{m}{\mathrm{Vol}}; \frac{d\vec{u}}{dt} + \tfrac{1}{\rho}\nabla\left(p+Q\right) = 0; \frac{de}{dt} + \tfrac{1}{\rho}\left(p+Q\right)\nabla\vec{u} = 0$$

or $$\frac{de}{dt} + \left(p+Q\right)\frac{dV}{dt} = 0$$

2. Figure out what mesh to remap to (*rezone*)
3. *Remap* the variable to the new zone

$$\frac{\partial\rho}{\partial t} = -\left(\vec{u} - \vec{u}_g\right)\nabla\rho; \frac{\partial\rho\vec{u}}{\partial t} = -\left(\vec{u} - \vec{u}_g\right)\nabla\rho\vec{u}; \frac{\partial\rho ue}{\partial t} = -\left(\vec{u} - \vec{u}_g\right)\nabla\rho e$$

4. Repeat

Lagrangian Equations

- **Lagrangian frame in integral form**

$$\frac{d}{dt}\int_{\Omega_t} \rho \, dv = 0 \quad \longrightarrow \quad \dot{\mathbf{x}} = \mathbf{u}$$

$$\frac{d}{dt}\int_{\Omega_t} \rho \dot{\mathbf{u}} \, dv = \int_{\Omega_t} \nabla \cdot (\mathbf{T} + \mathbf{T}^M) \, dv$$

$$\frac{d}{dt}\int_{\Omega_t} \rho e \, dv = \int_{\Omega_t} \mathbf{T} \cdot \nabla \mathbf{u} \, dv$$

$$\frac{d}{dt}\int_{\Gamma_t} \mathbf{B} \cdot \mathbf{n} \, dA = 0$$

Remesh-Remap

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}_g - \mathbf{u}$$

Remesh

$$\frac{\partial f_k}{\partial t} = -\left(\mathbf{u} - \mathbf{u}_g\right)\nabla f_k$$

$$\frac{\partial_r f_k \rho_k}{\partial t} = -\nabla \cdot \left(f_k \rho_k \left(\mathbf{u} - \mathbf{u}_g\right)\right.$$

$$\frac{\partial_\rho \mathbf{u}}{\partial t} = -\nabla \cdot \left(\rho \mathbf{u} \left(\mathbf{u} - \mathbf{u}_g\right)\right)$$

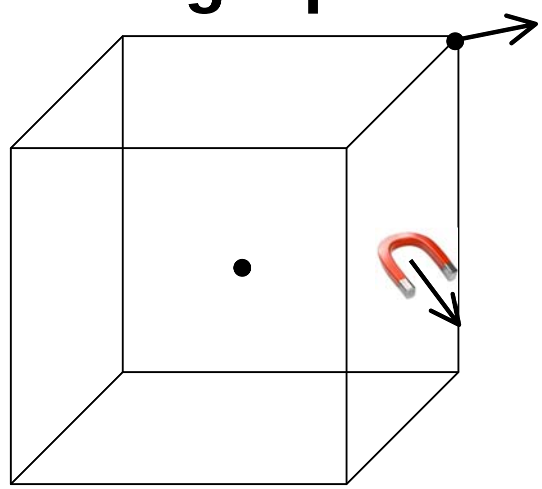
$$\frac{\partial_\rho e}{\partial t} = -\nabla \cdot \left(\rho e \left(\mathbf{u} - \mathbf{u}_g\right)\right)$$

$$\frac{\partial_\rho K}{\partial t} = -\nabla \cdot \left(\rho K \left(\mathbf{u} - \mathbf{u}_g\right)\right)$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \left(\mathbf{B} \times \left(\mathbf{u} - \mathbf{u}_g\right)\right) - \left(\mathbf{u} - \mathbf{u}_g\right)\left(\nabla \cdot \mathbf{B}\right)$$

Centering of Variables

- **Vertex-Face staggered grid (unstructured hexs)**
  - **Position, velocity, acceleration (nodal)**
  - **Density, energy, stress (element)**
  - **Magnetic field is face-centered**
  - **“Single point integration in space”**



Multimaterial Lagrangian Hydro

- When the elements have more than one material, the treatment is more complex.
- Two choices:
  – The classical equal volume treatment (argued to be unphysical)
  – A more modern treatment which allows the materials to treated as interacting adiabatically.

The modern multimaterial treatment

- **Assumes the materials are interacting adibatically. Could use a pressure relaxation as well.**
- **Changes the volume fraction and energy evolution**

$$\frac{df_k}{dt} = f_k \left(\frac{\bar{B}}{B_k} - 1 \right) \frac{\partial u}{\partial x}$$

$$f_k \rho_k \frac{de_k}{dt} = -f_k \frac{\bar{B}}{B_k} \bar{p} \frac{\partial u}{\partial x}$$

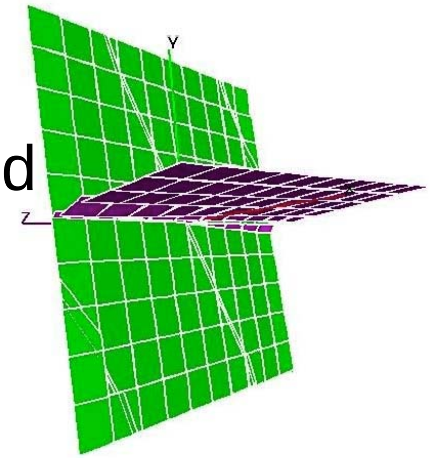
- **Requires more complicated average properties**

$$\bar{B} = \left(\sum_k \frac{f_k}{B_k} \right)^{-1} \qquad \bar{p} = \bar{B} \left(\sum_k \frac{f_k p_k}{B_k} \right)$$

Multimaterial Remap

- **The remap uses high resolution finite volume differencing for continuous fields**
- **Interface reconstruction with linearity preserving and automatic interface ordering (PIR) is used for discontinuous field (material interfaces).**

unsmoothed



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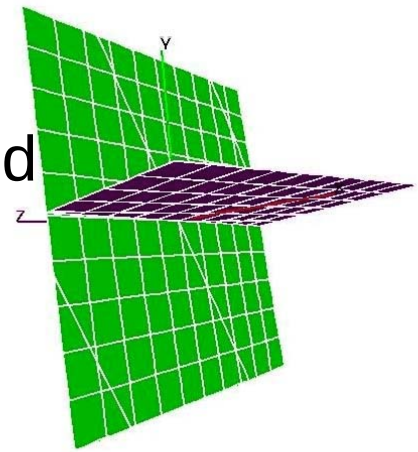


Multimaterial Remap

- **The remap process can create new mixed material elements which may be out of thermodynamic equilibrium.**
- **The elements should be brought into equilibrium before moving on from remap**
  - **This requires an adjustment of the volume fractions** $\Delta f_k = f_k \left(\frac{p_k - \bar{p}}{B_k} \right)$

$$f_k^1 = f_k^0 + \Delta f_k ; \rho_k^1 = \frac{f_k^0 \rho_k^0}{f_k^1} \qquad f_k^1 \rho_k^1 e_k^1 = f_k^0 \rho_k^0 e_k^0 - \bar{p} \Delta f_k$$

- **Any implementations requires limiters and renormalization** $f_k := \frac{f_k}{\sum_k f_k}$

$$\Delta f_k = \mathrm{sign}(\Delta f_k) \min\left(\Delta f_k, 0.1\right)$$

$$f_k := \max\left[0, \min\left(f_k, 1\right)\right]$$

Kinetic energy remap & total energy conservation

- **For some application (i.e. Z-pinch) this new feature is essential for good results.**
- **This adds a correction to the internal energy remap allowing energy conservation,** $K_{i,j,k} = \frac{1}{\mathrm{N}_{\mathrm{nodes}}} \sum_{\text{nodes of } i,j,k} 1/2\left(u^2+v^2+w^2\right)$

$$\Delta e_{i,j,k}^{\text{remapped}} = \left(K_{i,j,k}^{\text{remapped}} - \frac{1}{\mathrm{N}_{\mathrm{nodes}}} \sum_{\text{nodes of } i,j,k} 1/2\left(u^2+v^2+w^2\right)^{\text{remapped}} \right)$$

$$q_j/p_j < 0.0001 \text{ set } \Delta e_{i,j,k}^{\text{remapped}} = 0$$

$$\Delta e_{i,j,k}^{\text{remapped}} < -\beta e_{i,j,k}^{\text{remapped}},\ \Delta e_{i,j,k}^{\text{remapped}} = -\beta e_{i,j,k}^{\text{remapped}}$$

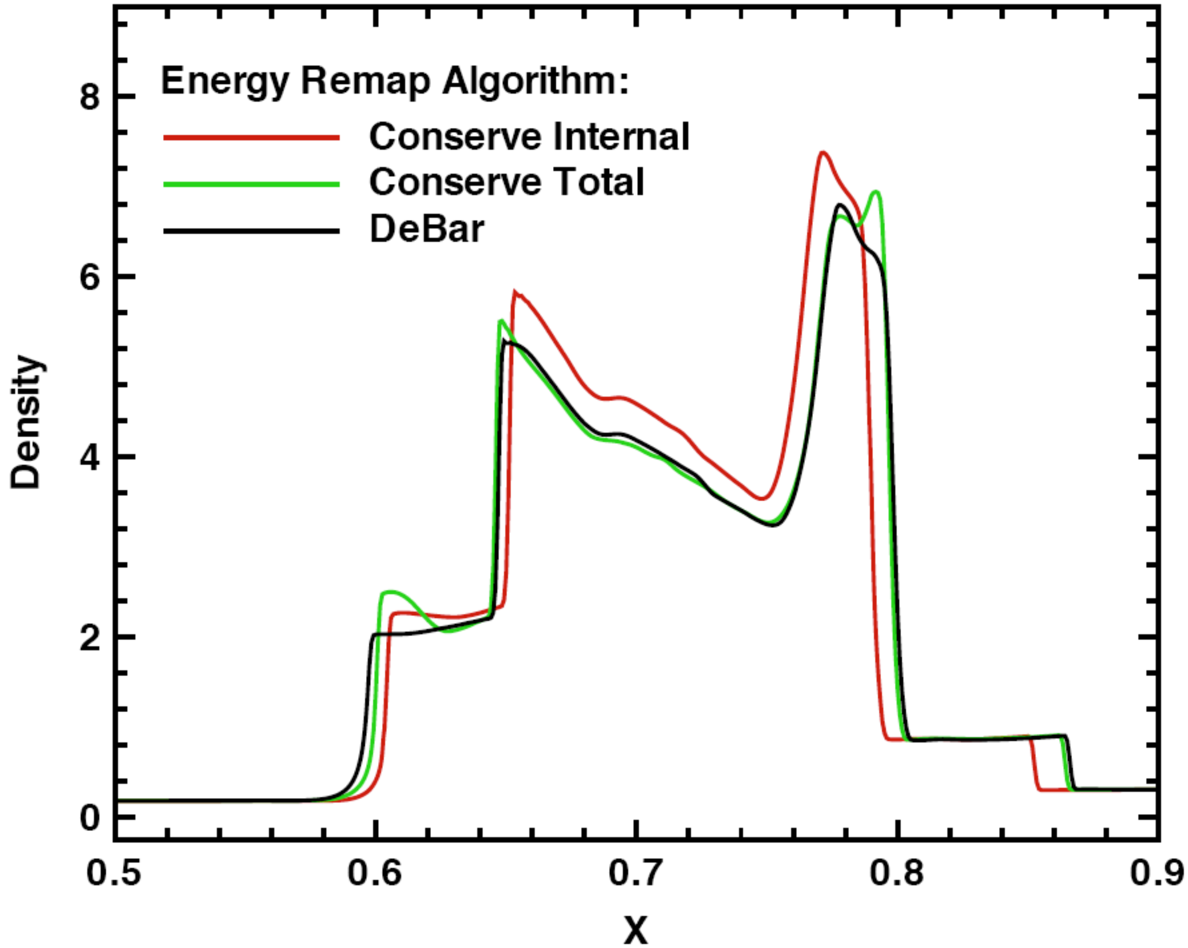
- **“fixes” are necessary for robust use!**

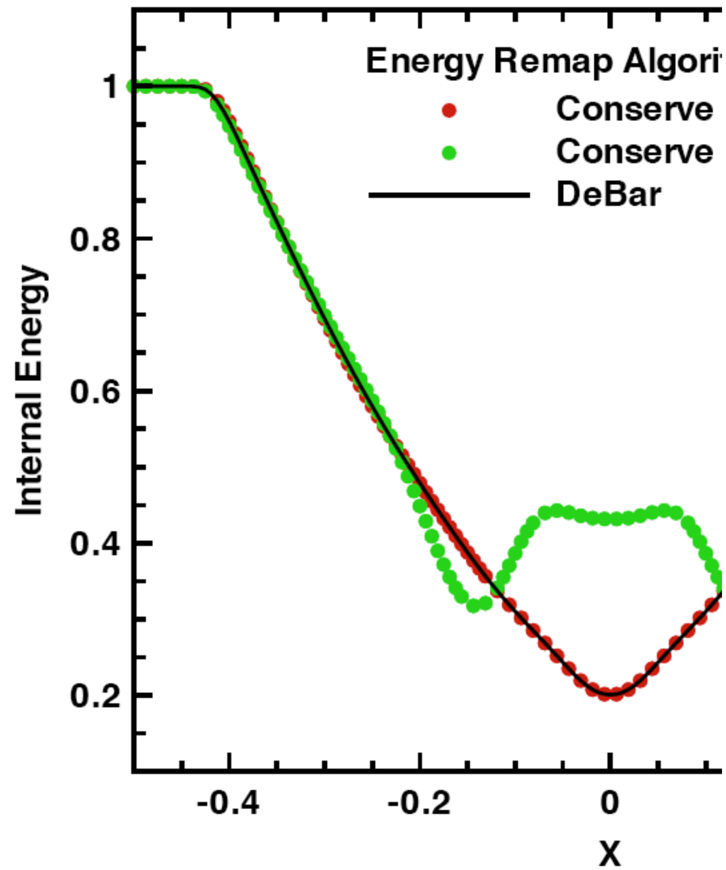
MHD

- Uses a compatible formulation that preserves the divergence free magnetic field automatically.
- A software package, Intrepid, makes the implementation relatively seamless
- These properties are important to maintain through the remap as well.
- ALEGRA includes magnetic diffusion as well as ideal MHD

Applications: Verification

- **Classic compressible flow problems (we're also studying ideal MHD flows!)**





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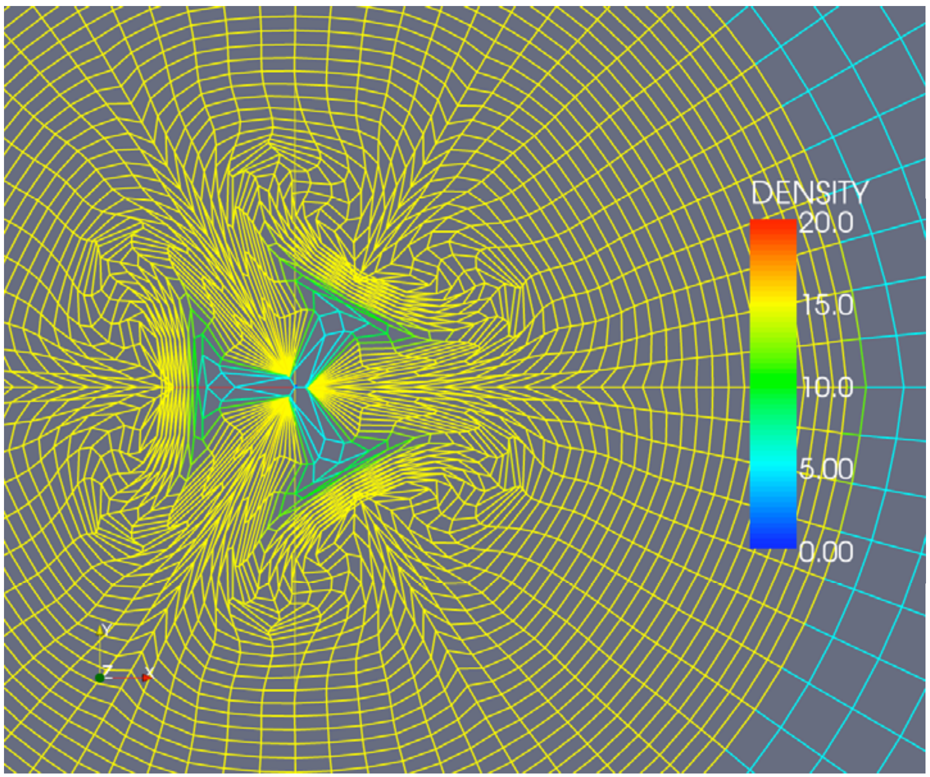
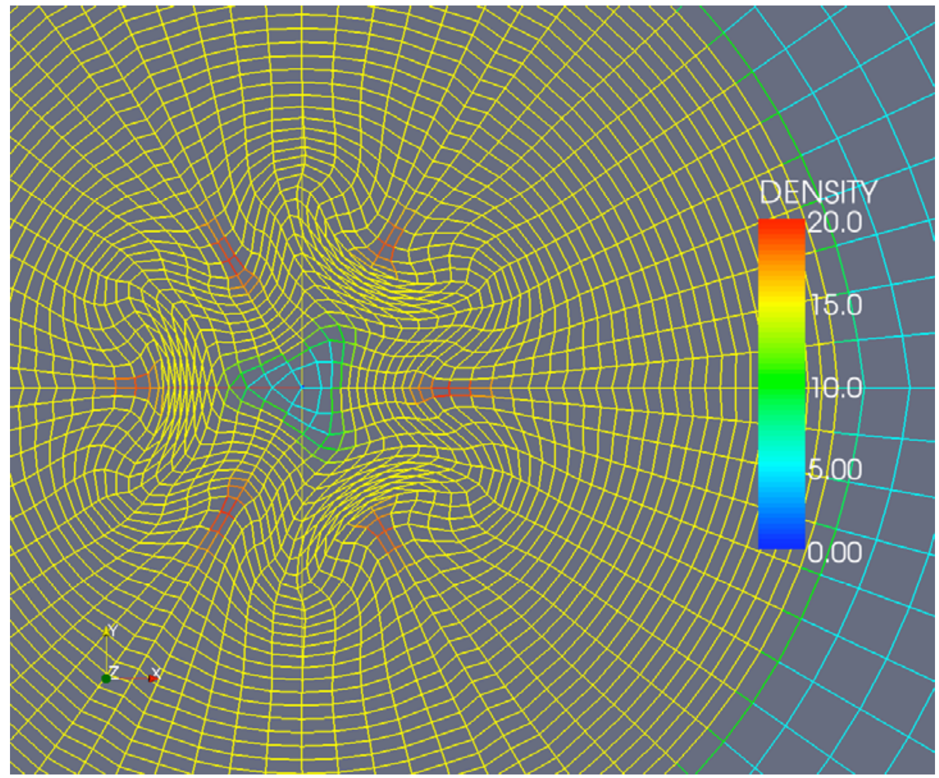
Cylindrical Noh Results

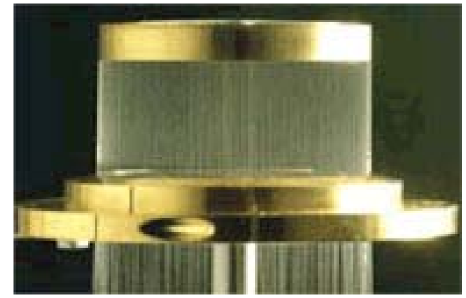
Scalar Q



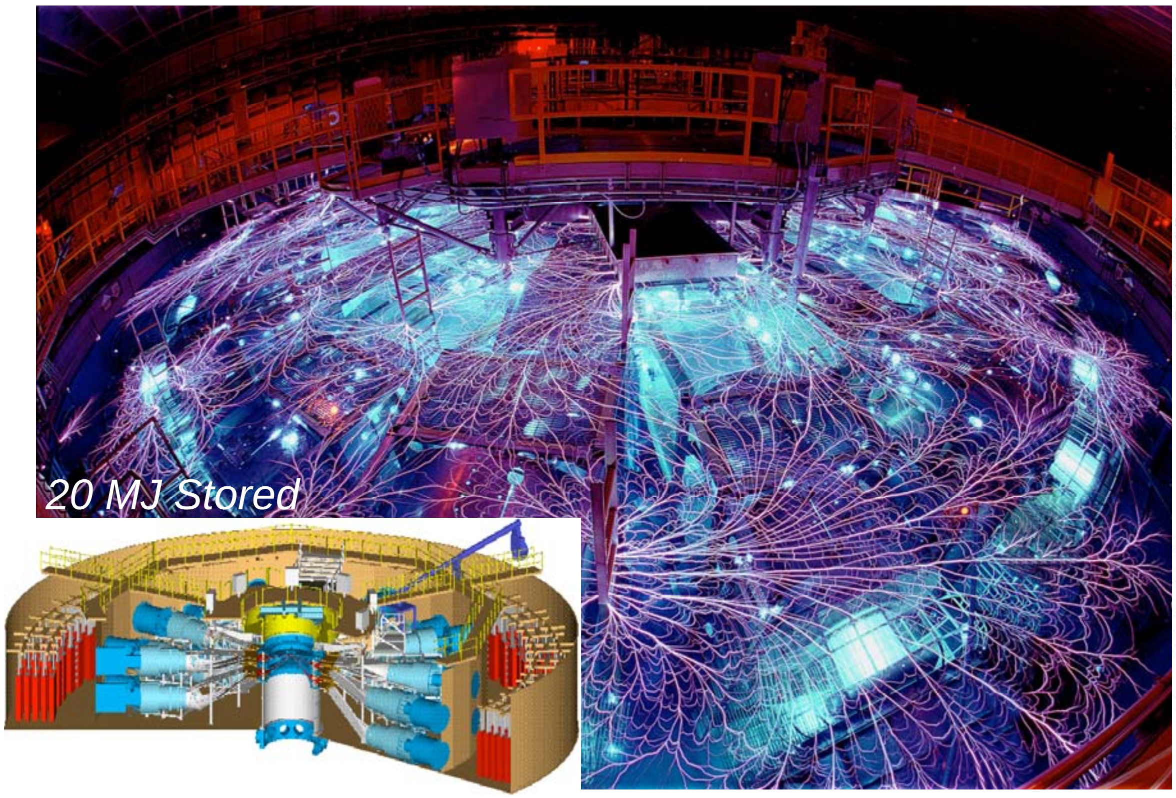
Tensor Q



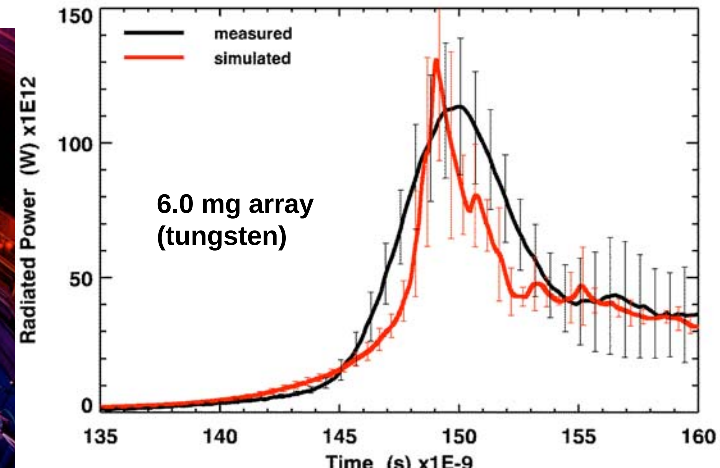
Applications: Z-Pinch

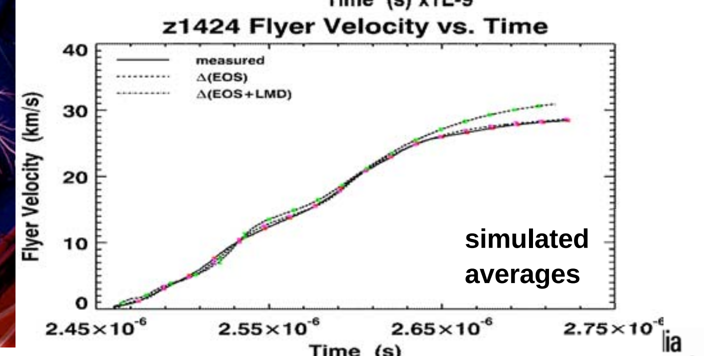


- **ALEGRA has provided predictive simulations of magnetic flyers and wire array implosions conducted on SNL’s Z-machine.**



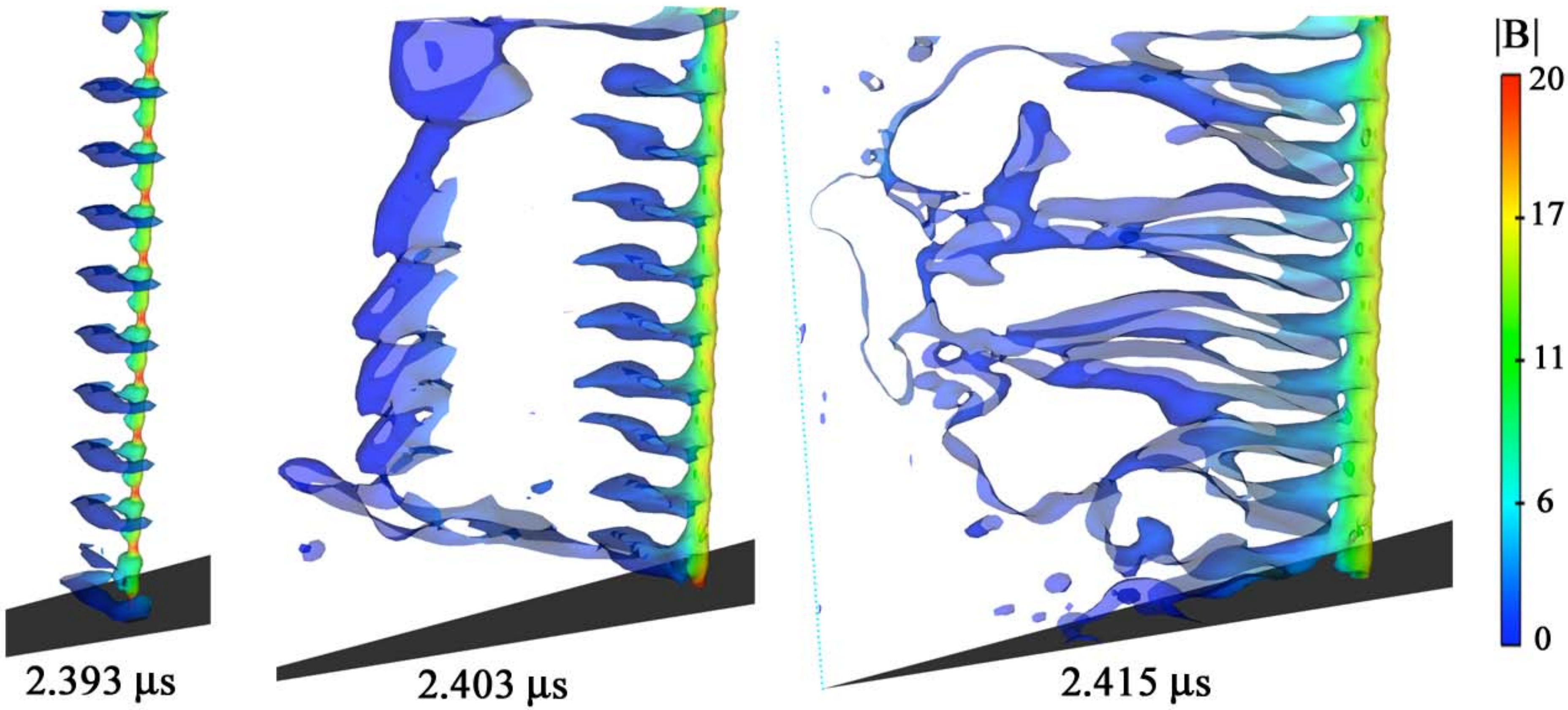
Radiated Power vs. Time





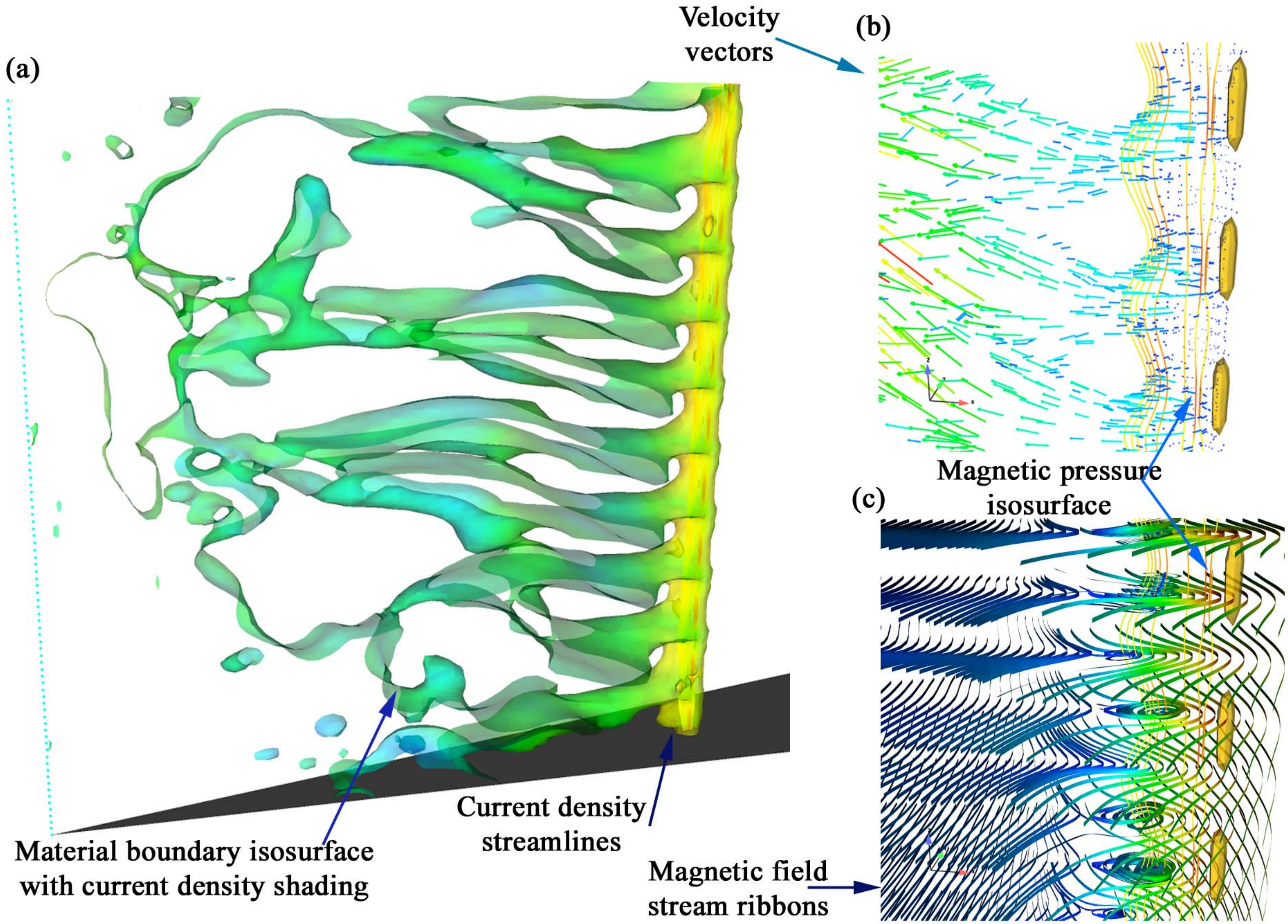
Sinusoidal Core Perturbation

Volume fraction isosurface with magnetic field strength



- Is this a variation of the m=0 instability for wire arrays?

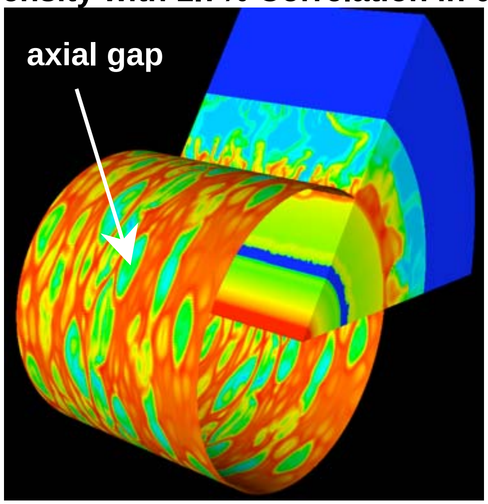
- Are the local dynamics governed by the the strength of the local field versus the global?

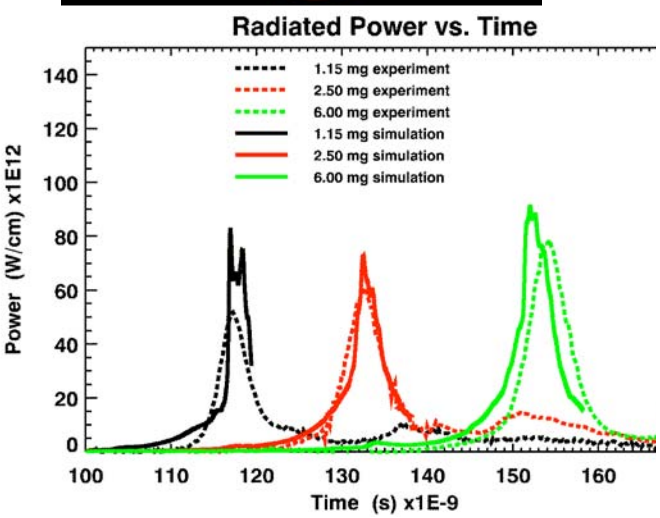


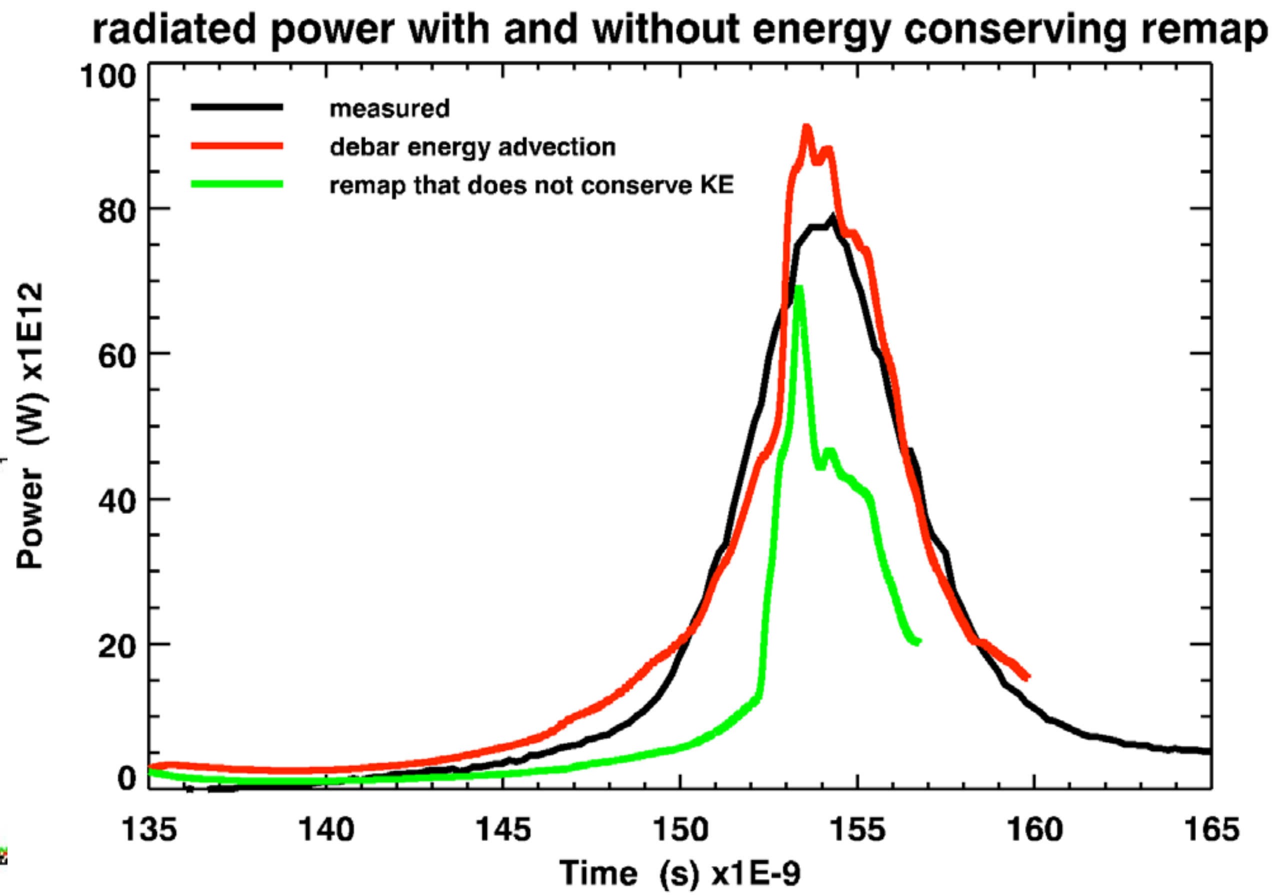
(a)
(b)
(c)
Velocity vectors
Magnetic pressure isosurface
Current density streamlines
Material boundary isosurface with current density shading
Magnetic field stream ribbons

Wire Array Implosions require 3-D and all the physics!

Density with 1.7% Correlation in θ







Simulates a wide range of parameters

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Applications: Advanced Material Modeling

- Material modeling is important in many applications such as armor or anti-armor simulations.
- Among the most difficult aspect is fracture modeling which tends to be strongly size dependent –
  - Does not easily allow mesh independence
- ALEGRA has addressed this!

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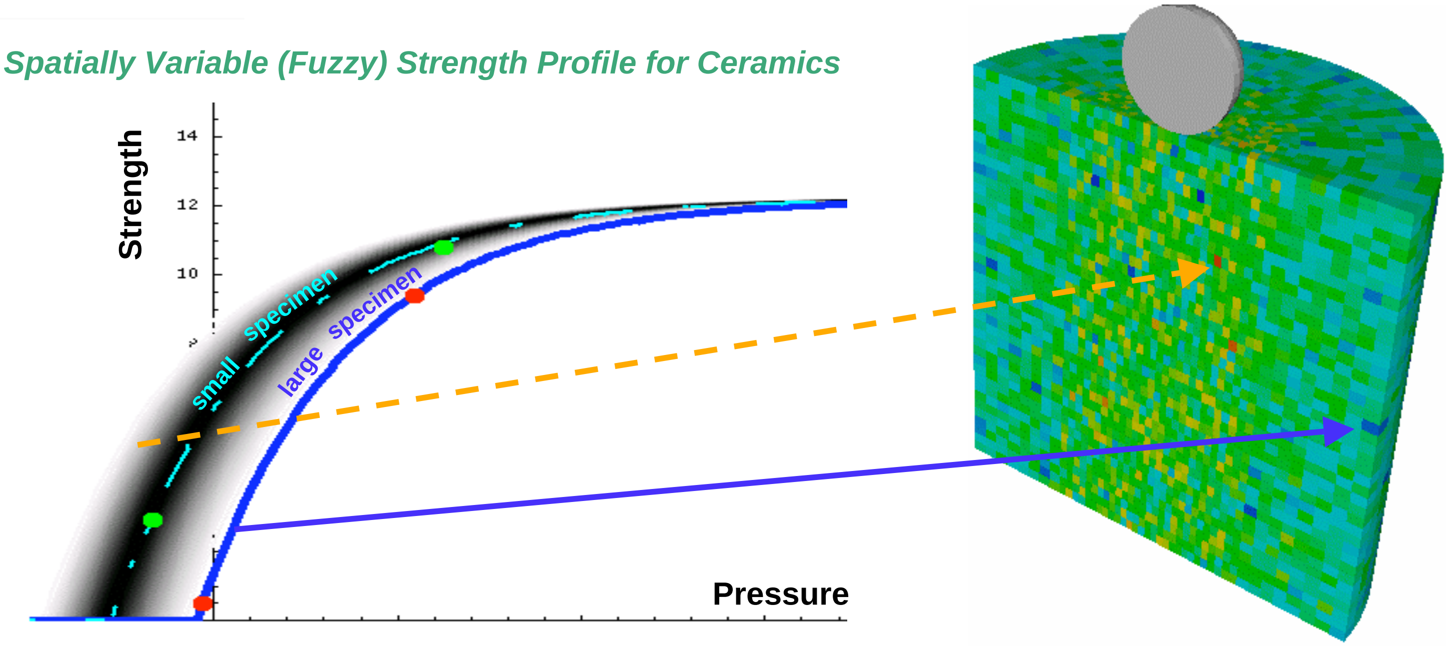
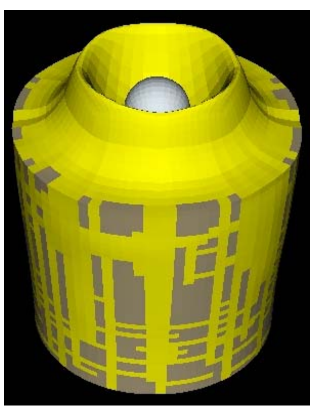
Brannon, Strack

Material Heterogeneity is Crucial when Simulating Failure in Armor Systems

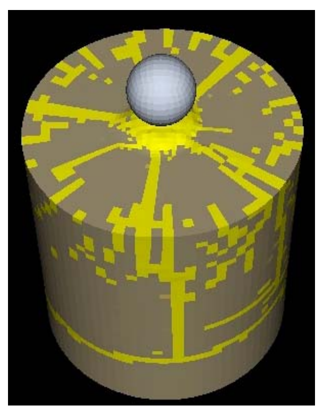
Spatially Variable (Fuzzy) Strength Profile for Ceramics



Initial state: small elements are stronger on average, but also more variable



Without Variability



With Variability

Key Collaboration: Brannon, University of Utah

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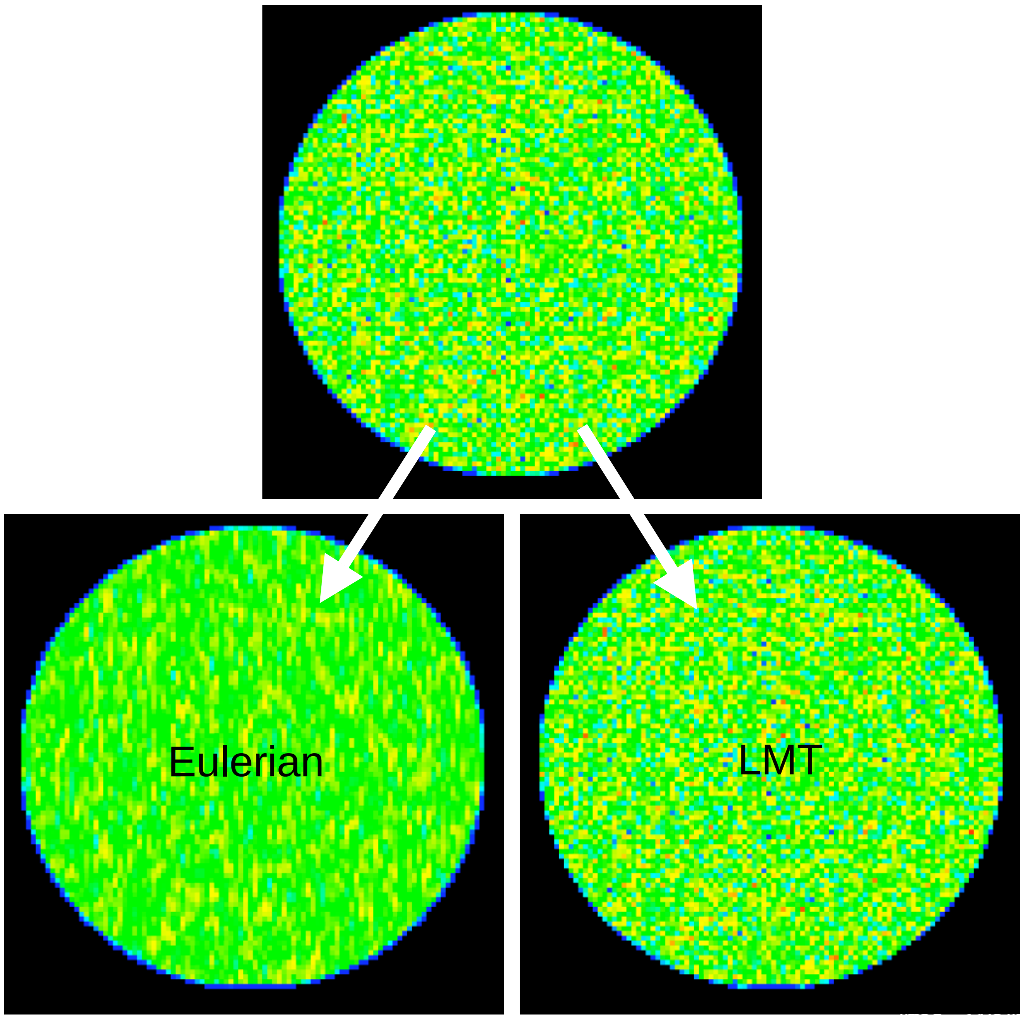
LMT Eliminates Smearing of Heterogeneity in Conventional Eulerian Algorithms

Initial State

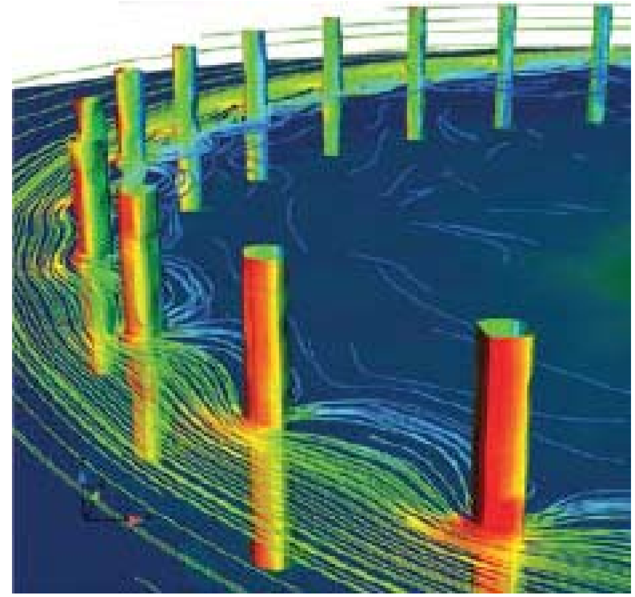


After Remap

Lagrangian Material Tracking (LMT):

- **Standard Eulerian momentum solver**
- **Material internal state variables reside on Lagrangian tracers**

Conclusions



- ALEGRA is a complex multiphysics code developed at SNL principally under the ASC program
- It has multimaterial capability
- MHD is an important aspect of many applications for ALEGRA
- Applications demonstrated are Z-pinch dynamics and complex material modeling.

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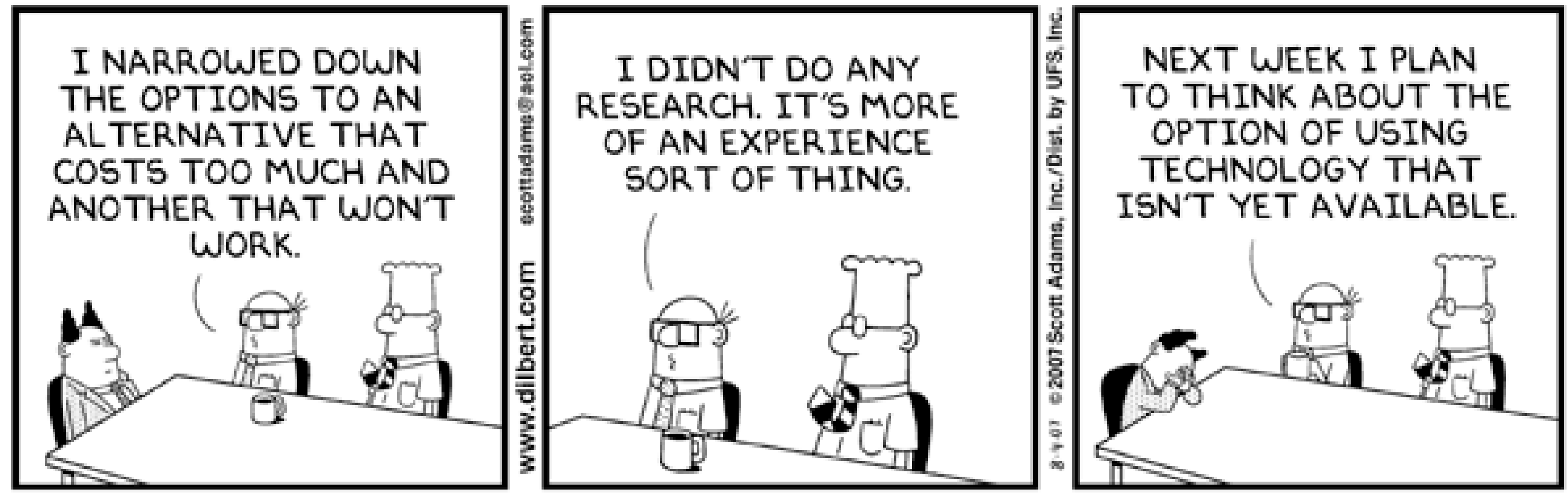
Scott Adams has an observation



"For the numerical analyst there are two kinds of truth; the truth you can prove, and the truth you see when you compute." – Ami Harten