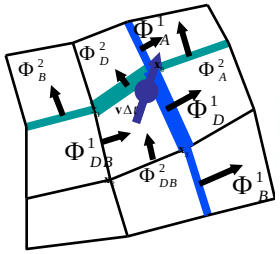
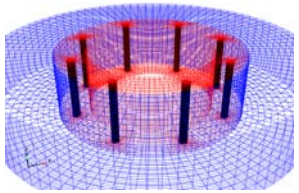
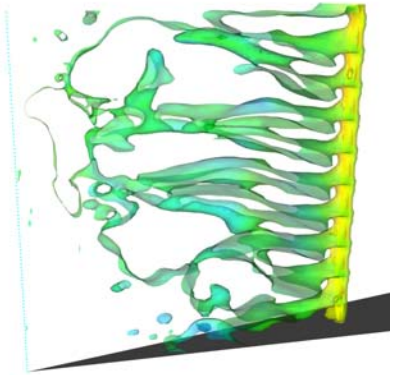
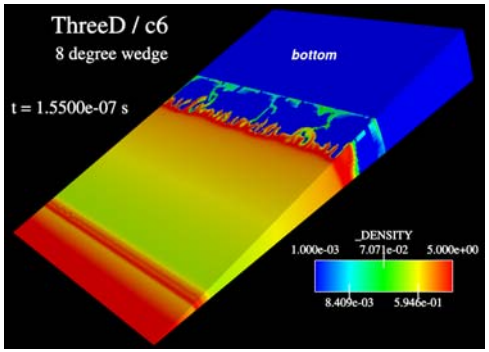
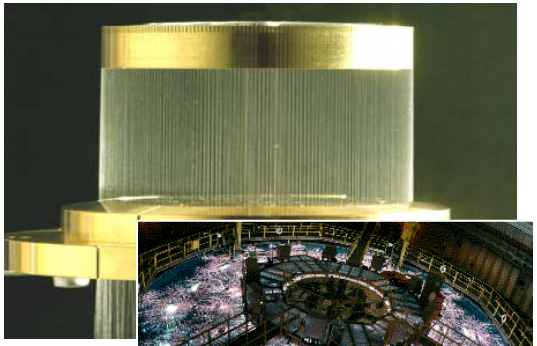
Multimaterial ALE algorithms in ALEGRA

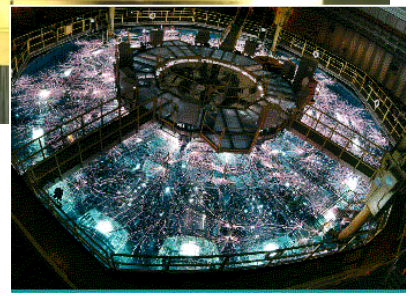












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Sandia National Laboratories, Albuquerque, NM

ALE from ART to SCIENCE
Los Alamos National Laboratory
June 10-13, 2008

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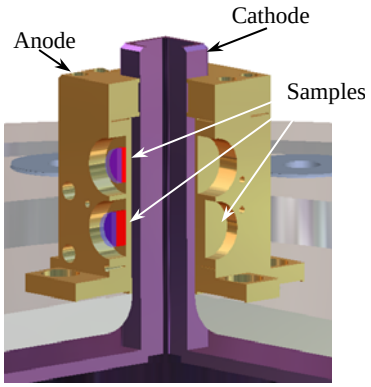
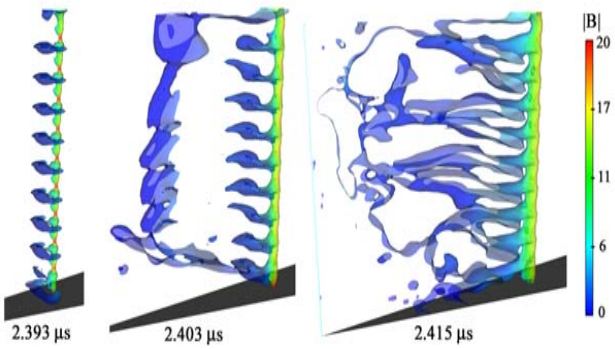
Outline

- Flyer Application
- Strategic Directions
- Algorithm areas:
  - Multi-material Lagrangian
  - Remesh methodologies
  - Remap methodologies
    - Hydro
    - MHD
    - Solid kinematics
    - Lagrangian Material Tracking
    - Energy conservation
- Summary





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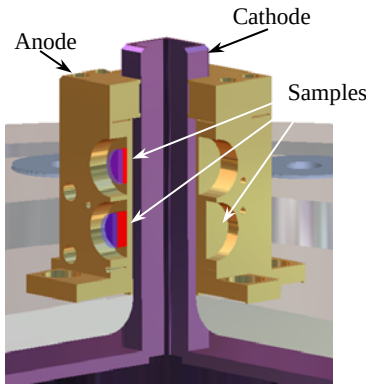
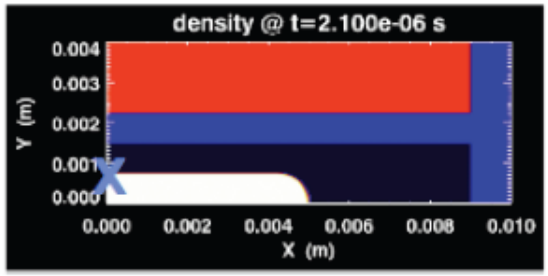
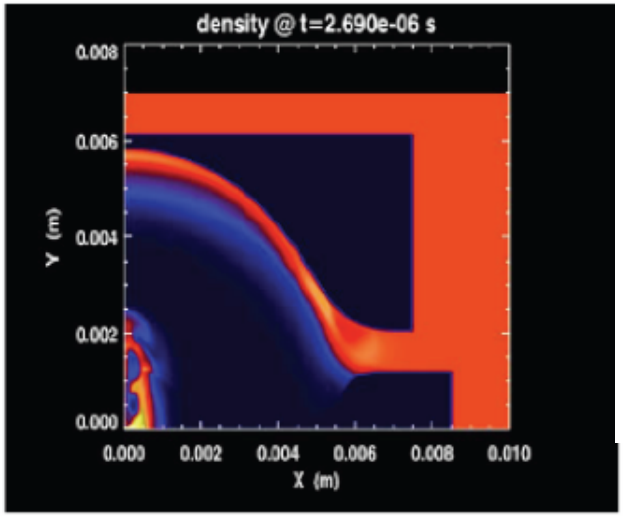
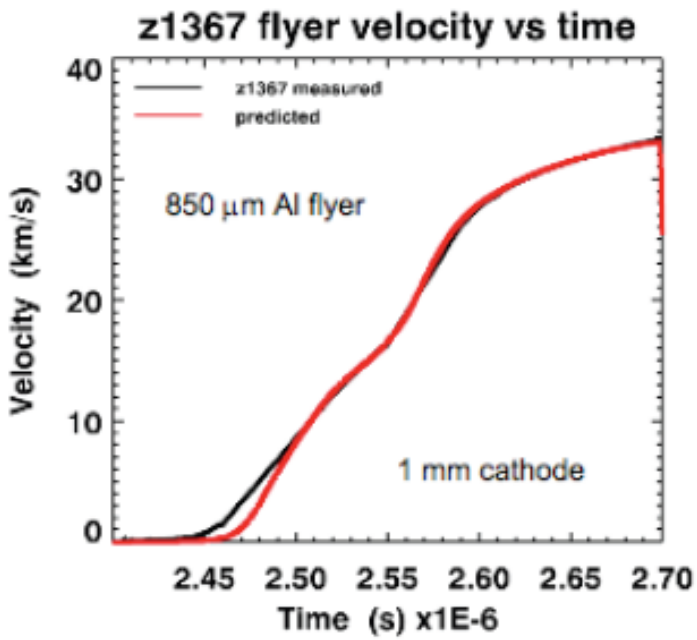
Flyer Application









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Definitions

- **Lagrangian:**
  - Mesh moves with material points.
  - Mesh-quality may deteriorate
- **REMESH**
  - Mesh-quality is adjusted to improve solution-quality or robustness.
  - Eulerian sets new mesh to original location
- REMAP
  - algorithm transfers dependent variables to the new mesh.

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Multi-material Lagrangian

- ALE implies a discussion of multimaterial Lagrangian treatments.
- The Lagrangian hydro algorithm in ALEGRA is based on the method from the SNL code PRONTO.
- It uses the Von Neumann-Richtmyer time-space staggering, but the energy equation is first-order in time; however the method is conservative.
  - It's the "same" as the predictor in the compatible P-C method, except for the time-centering.
  - Unfortunately, this approach has an expansion instability.
- We are moving as quickly as possible to a full predictor corrector scheme to enable energy conservation and stability.
- We are in the process of investigating a FEM compatible limited Q using a least square approach to computing a limiter.

ALEGRA mixed element treatments

ALEGRA has historically implemented a constant volume fraction with a volume fraction averaged stress method

$$\frac{df_k}{dt} = 0 \qquad \bar{p} = \sum_k f_k p_k \qquad p_k = P(\rho_k, e_k)$$

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Working on more realistic multi-material treatment(s)

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

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

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Algorithmic modifications are required for a robust algorithm

- **Large changes in material volume are dangerous and must be limited, however**
- **Not allowing enough of a change keeps materials in unphysical states (doesn't allow appropriate adjustment).**
- **The dangerous changes are associated with being nearly full or empty. For each material**

$$\alpha_m = \begin{cases} \min\left(1.0, -0.05/\left(\delta f / f\right), -0.25/\left(\delta f /(1-f)\right)\right) \ , \ \delta f < 0 \\ \min\left(1.0, 0.05/\left(\delta f /(1-f)\right), 0.25/\left(\delta f / f\right)\right) \end{cases}$$

$$\delta f_{new} := \min(\alpha_m)\delta f$$

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ALEGRA Remesh Requirements

- Mesh connectivity will remain fixed
- Local remapping (Courant condition)
- Unstructured grids (QUAD4/HEX8)
- Minimal user involvement with intuitive controls.
- External and internal boundary constraints must be handled.
- Large scale parallel algorithm must achieve mesh decomposition independent results.
- Robust.
- Reasonable CPU cost.

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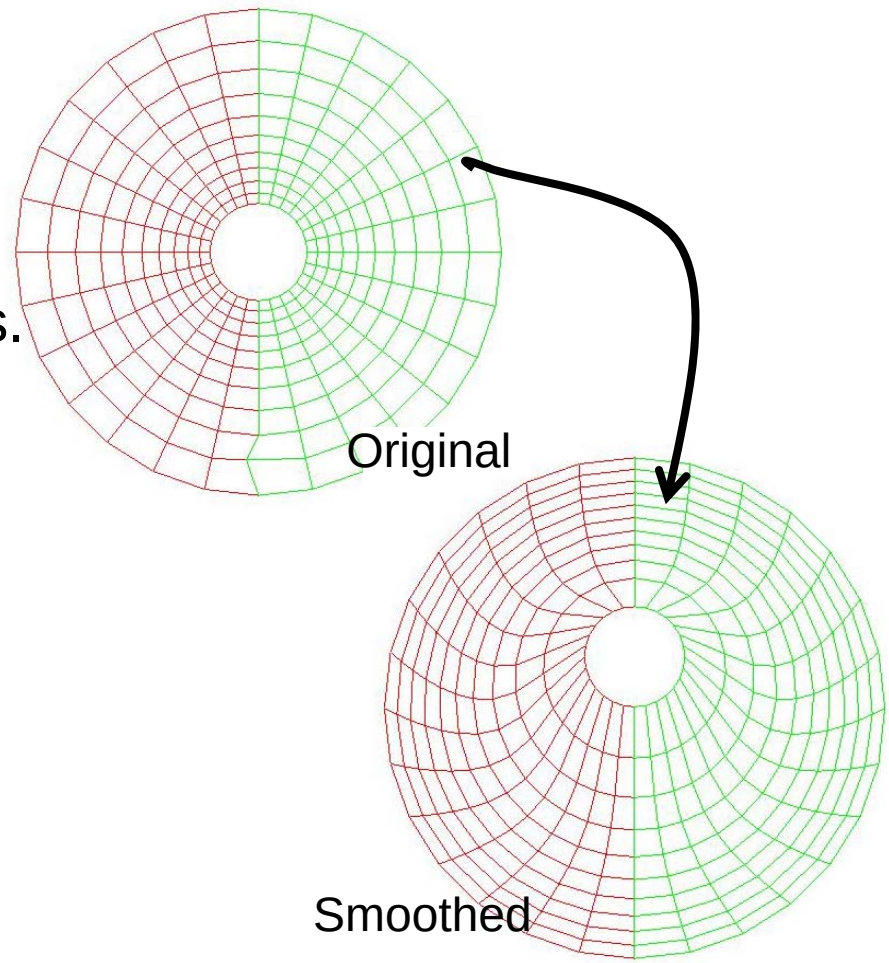
Early Efforts

- Based on a weighted Winslow type method (equipotential).
- Suitable for unstructured meshes.
- Computationally efficient.
- Only limited control of element quality.
- Non-intuitive user interaction/tweaking



ALE did not gain much traction in ALEGRA's user community.

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Current Efforts

- New remesh is based on MESQUITE Mesh Improvement Library (See talk by Knupp this workshop).
  - Wide range of mesh improvement algorithms.
  - Reference metric methods.
    - Allows user to specify a “target-mesh.”
    - Might be used in conjunction with knowledge of solution to construct physics-aware mesh-improvement.
    - Plethora of “reference-mesh” options available...
  - Significant experience in mesh-generation (e.g. CUBIT).
  - Limited usage in hydro-codes.
- ALEGRA is using a modified version of MESQUITE 0.9.6 (Mike Brewer) to achieve its remesh requirements.

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Mesquite Remesh: Underlying Methodology

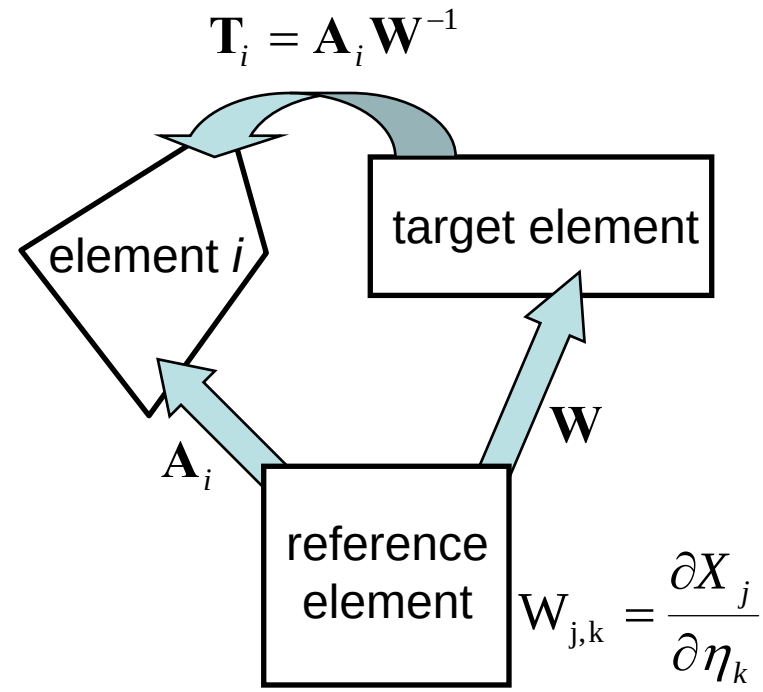
- Define an element quality metric -

$$\mu_i = \frac{\| \mathbf{T}_i \|_F^2}{\det \mathbf{T}_i^{\,a}}$$

- Write objective function -

$$F_{\mu,\hat{\Omega}} = \sum_{i \in \hat{\Omega}} \mu_i^{\,p}$$

- Minimize *F* w.r.t. vertex locations.



A significant issue for our applications is the appropriate selection of a target element (i.e. **W**) and quality metric.

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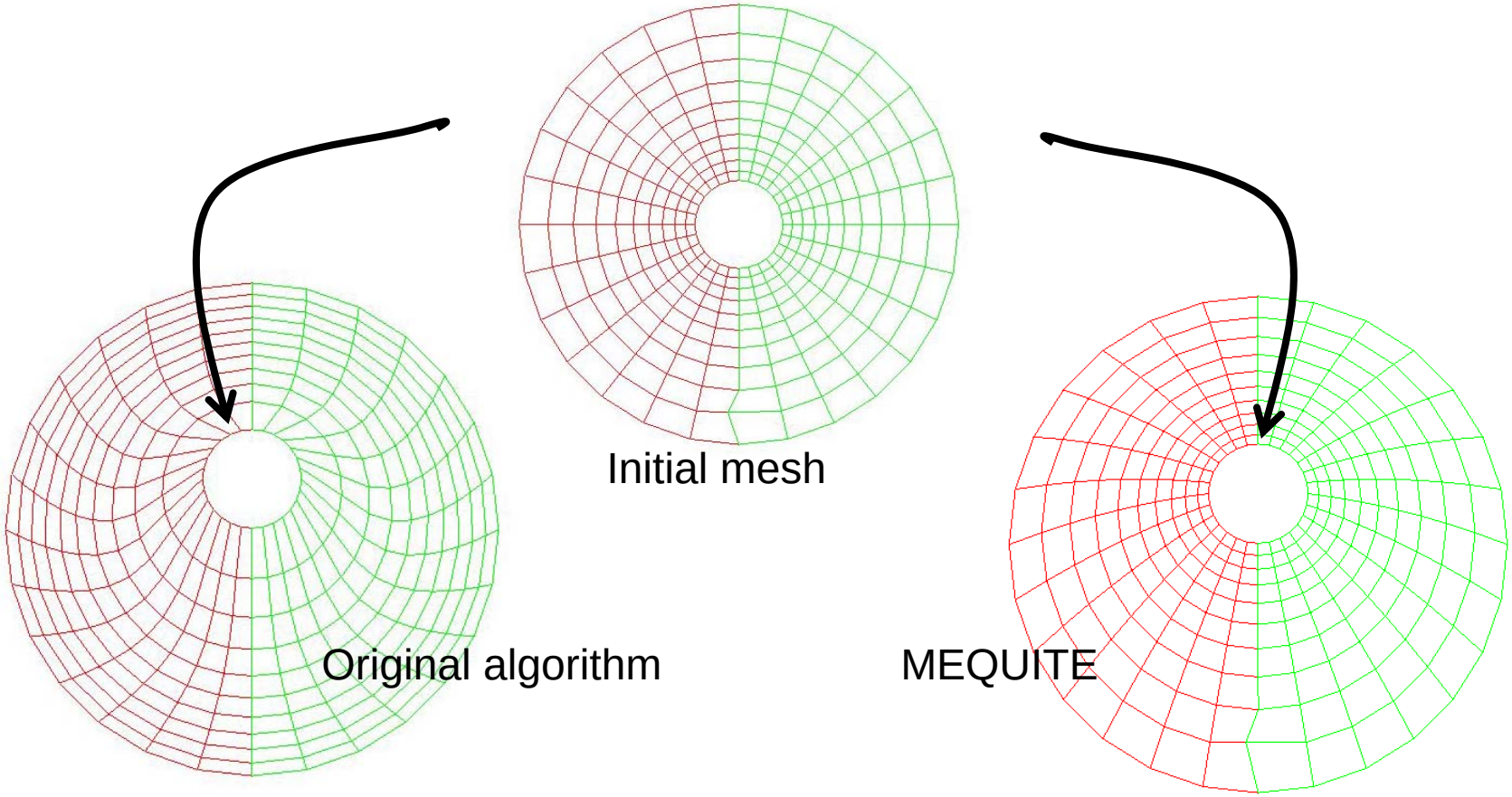
ALEGRA Implementation Details

- Parallel:
  - Jacobi-style iteration. Easy to implement, preserves symmetries.
- Metric:
  - Inverse Mean Ratio
- Target element:
  - Initial or ideal mesh target calculators.
- Boundary conditions for planar surfaces:
  - The closest-point projection was problematic.
  - Implementing a reflected boundary element about surface ensured optimal convergence and maintained symmetry.

A Comparison of Equipotential and MESQUITE Meshes



MESQUITE implementation preserves mesh grading without additional controls.

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Current Capabilities

- Domain Smoothing:
  - Weighted Winslow
  - Mesquite (Inverse mean ratio works best)
- Boundaries (internal/external) Smoothing:
  - Planar smoothing with reflected boundaries
  - Lagrangian
  - Eulerian
- Controls:
  - Target initial or ideal element (MESQUITE).
  - Node movement limiting (respect Courant limit).
  - Number of Jacobi solver iterations.

Remap

- Eulerian style remesh/remap usage is very common with ALEGRA users.
- Remap Overview Summary
  - Interface reconstruction options.
  - Remap algorithms:
    - Hydro
    - MHD
    - Solid kinematics
  - DeBar modifications to kinetic and magnetic energy to support shocks.

Interface Reconstruction Options

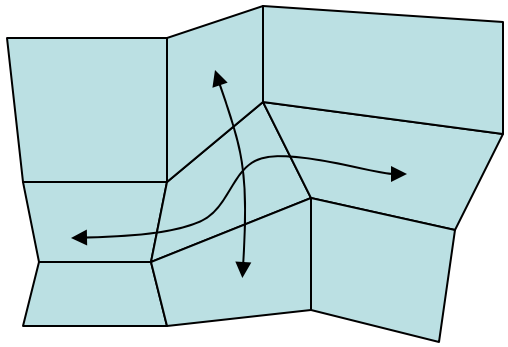
- SLIC – Single Line Interface Reconstruction

- SMYRA – Sandia Modified Young's Reconstruction works with a unit cube description and has an automatic ordering algorithm.
- New SMYRA – Alternate version of SMYRA algorithm

- PIR – Patterned Interface Reconstruction
  - Works with physical element description (not unit cubes)
  - Additional smoothing steps yields second order accuracy
  - Strict ordering and polygonal removal by material guarantees self-consistent geometry.
  - 2D arcs are implemented.
  - 3D spherical caps are planned.
  - Jay Mosso will give details in Wednesday presentation.

ALEGRA Hydro Remap Summary

- **Element based reconstruction operators utilize one-dimensional mesh topology associated stencils (quads and hexes). Volume or mass coordinates are used.**
- **Momentum remapped using half-interval shift.**



- **It is desirable to replace this split remap methodology. An unsplit remap algorithm for hydro is in progress.**

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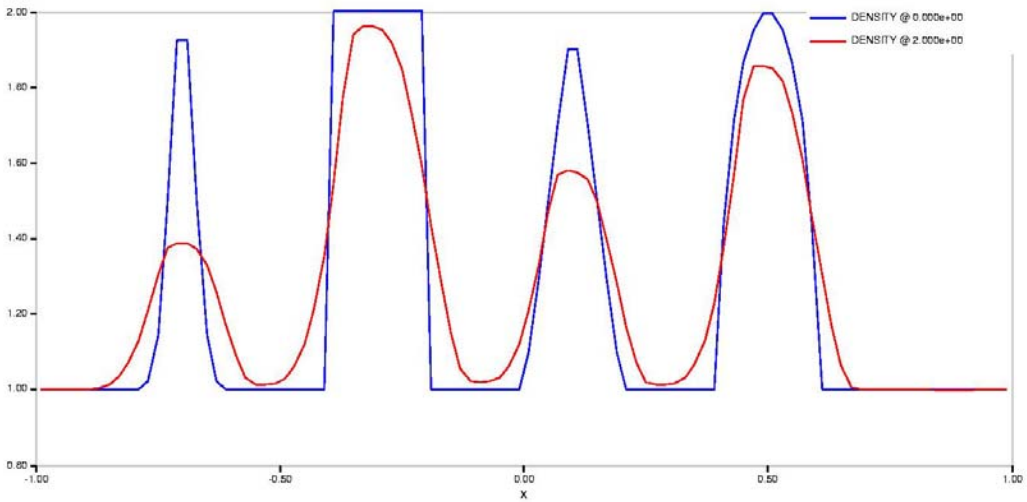
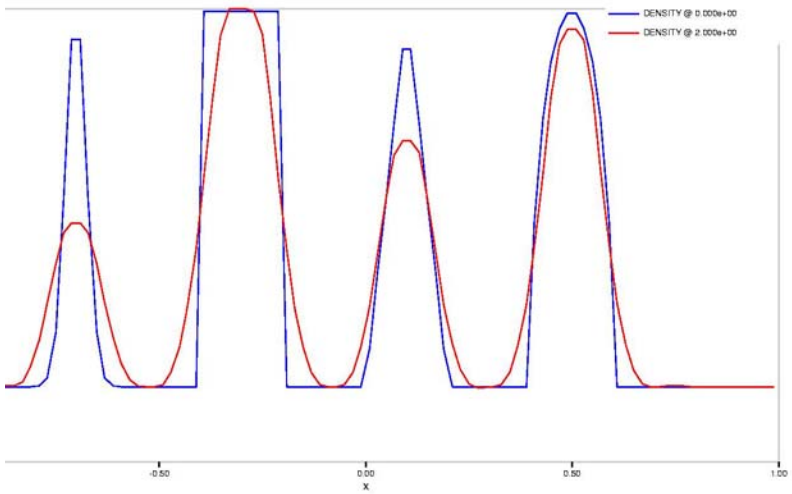
Hydro Remap Improvements

- **Remap methods have been improved with an improved van Leer method on variable meshes and a third-order scheme.**



Standard van Leer



3rd Order

- **These new methods are still being evaluated on applications.**

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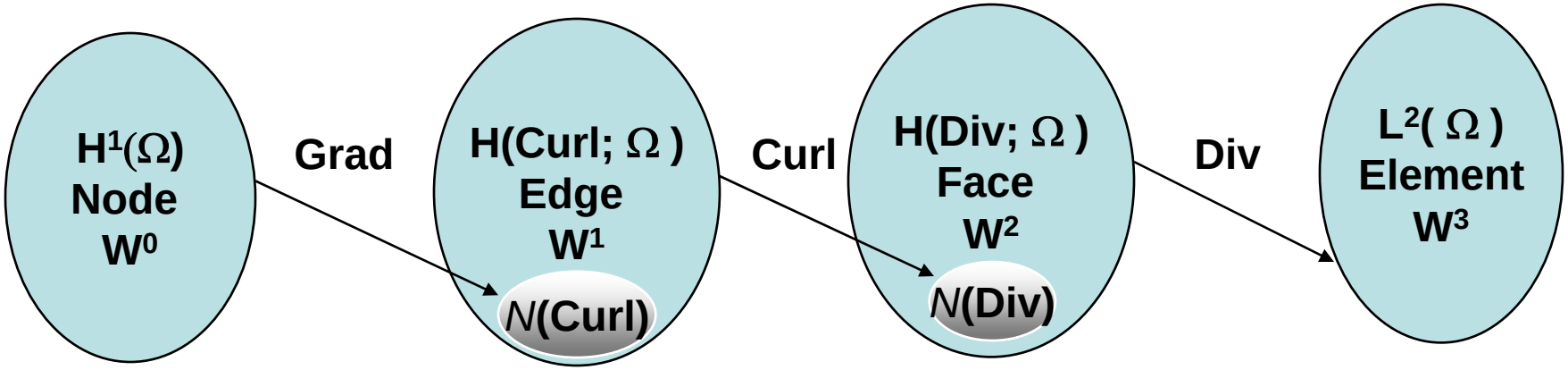
Mimetic discretizations (deRham complex) are natural for MHD



- Magnetic flux and vector potential circulation are invariants in ideal MHD and thus natural degrees of freedom.
- Circulation is the degree of freedom for the edge element.
- Flux in the degree of freedom for the face element.
- Discrete node, edge, face element representations matching these properties are possible using mimetic FE to solve the magnetic diffusion equation in an operator split context.
- In 3D we thus ensure that fluxes exactly satisfy the divergence free property for the magnetic flux density.

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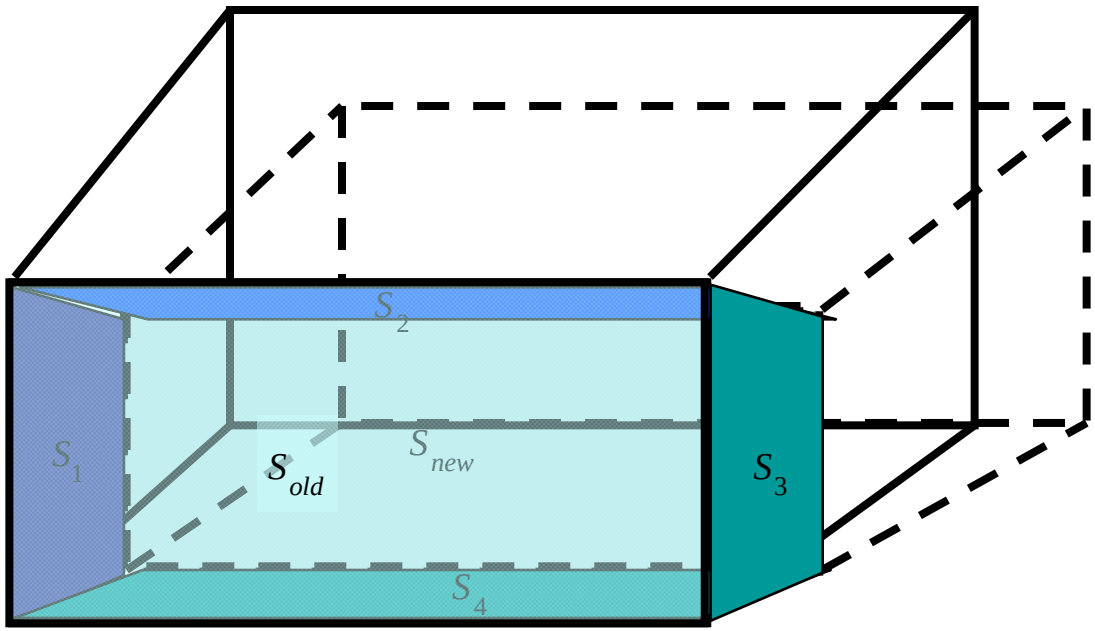
Magnetic Flux Density Remap

- 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.

Flux remap step

$$\int_S \mathbf{B} \bullet d\mathbf{a} = 0$$

$$\int_{S_{old}} \mathbf{B} \bullet d\mathbf{a} + \int_{S_{new}} \mathbf{B} \bullet d\mathbf{a} + \sum_{i=1}^{4} \int_{S_i} \mathbf{B} \bullet (\mathbf{v}_g \Delta t \times \mathbf{dl}) = 0$$



$$\int_{S_{old}} \mathbf{B} \bullet d\mathbf{a} + \int_{S_{new}} \mathbf{B} \bullet d\mathbf{a} + \sum_{i=1}^{4} \int_{S_i} \mathbf{dl} \bullet (\mathbf{B} \times \mathbf{v}_g \Delta t) = 0$$

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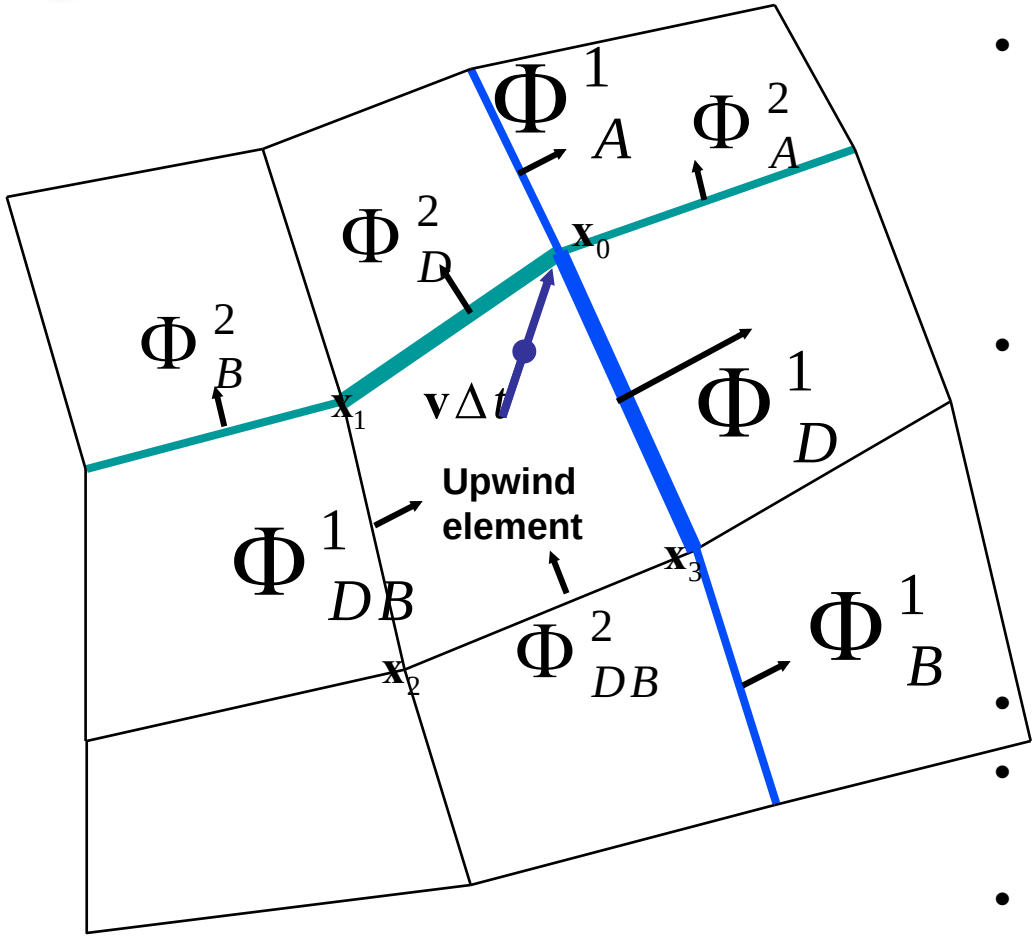
CT on unstructured quad and hex grids (CCT)



- **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 red 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.**

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Face element representation

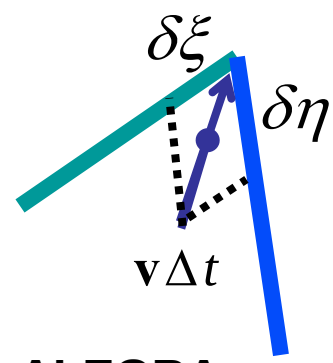
- **Obtain representation of upwind element in terms of natural coordinates of an isoparametric element.**

$$\mathbf{x} = (\mathbf{x}_0 + \xi(\mathbf{x}_1 - \mathbf{x}_0)) + \eta[(\mathbf{x}_3 + \xi(\mathbf{x}_2 - \mathbf{x}_3)) - (\mathbf{x}_0 + \xi(\mathbf{x}_1 - \mathbf{x}_0))]$$

$$\mathbf{B} = \sum_f \Phi_f \mathbf{F}_f = \frac{\Phi_D^1(\xi - 1)\frac{\partial \mathbf{x}}{\partial \xi}}{\frac{\partial \mathbf{x}}{\partial \xi} \times \frac{\partial \mathbf{x}}{\partial \eta}} + \frac{-\Phi_{DB}^1 \xi \frac{\partial \mathbf{x}}{\partial \xi}}{\frac{\partial \mathbf{x}}{\partial \xi} \times \frac{\partial \mathbf{x}}{\partial \eta}} + \frac{\Phi_D^2(\eta - 1)\frac{\partial \mathbf{x}}{\partial \eta}}{\frac{\partial \mathbf{x}}{\partial \xi} \times \frac{\partial \mathbf{x}}{\partial \eta}} + \frac{-\Phi_{DB}^2 \eta \frac{\partial \mathbf{x}}{\partial \eta}}{\frac{\partial \mathbf{x}}{\partial \xi} \times \frac{\partial \mathbf{x}}{\partial \eta}}$$

- **Integrate over flux surface.**

$$\int_{S_i} d\mathbf{x} \times \mathbf{B} \approx \delta\eta(\Phi_D^1 + \tfrac{\delta\xi}{2}(\Phi_{DB}^1 - \Phi_D^1)) - \delta\xi(\Phi_D^2 + \tfrac{\delta\eta}{2}(\Phi_{DB}^2 - \Phi_D^2))$$



- **Normal gradient terms appear naturally.**

•A cross face tangential gradient limiting analogous to the ALEGRA geometry independent reconstruction is implemented and EH ideas for Cartesian grids

•Several limiters implemented (Van Leer, harmonic, minmod, donor)

$$\widehat{\Phi}^1(\eta) = \Phi_D^1 + (A_D^1)^2 s^1(\tfrac{1}{2} - \eta) \qquad \widehat{\Phi}^2(\xi) = \Phi_D^2 + (A_D^2)^2 s^2(\tfrac{1}{2} - \xi)$$

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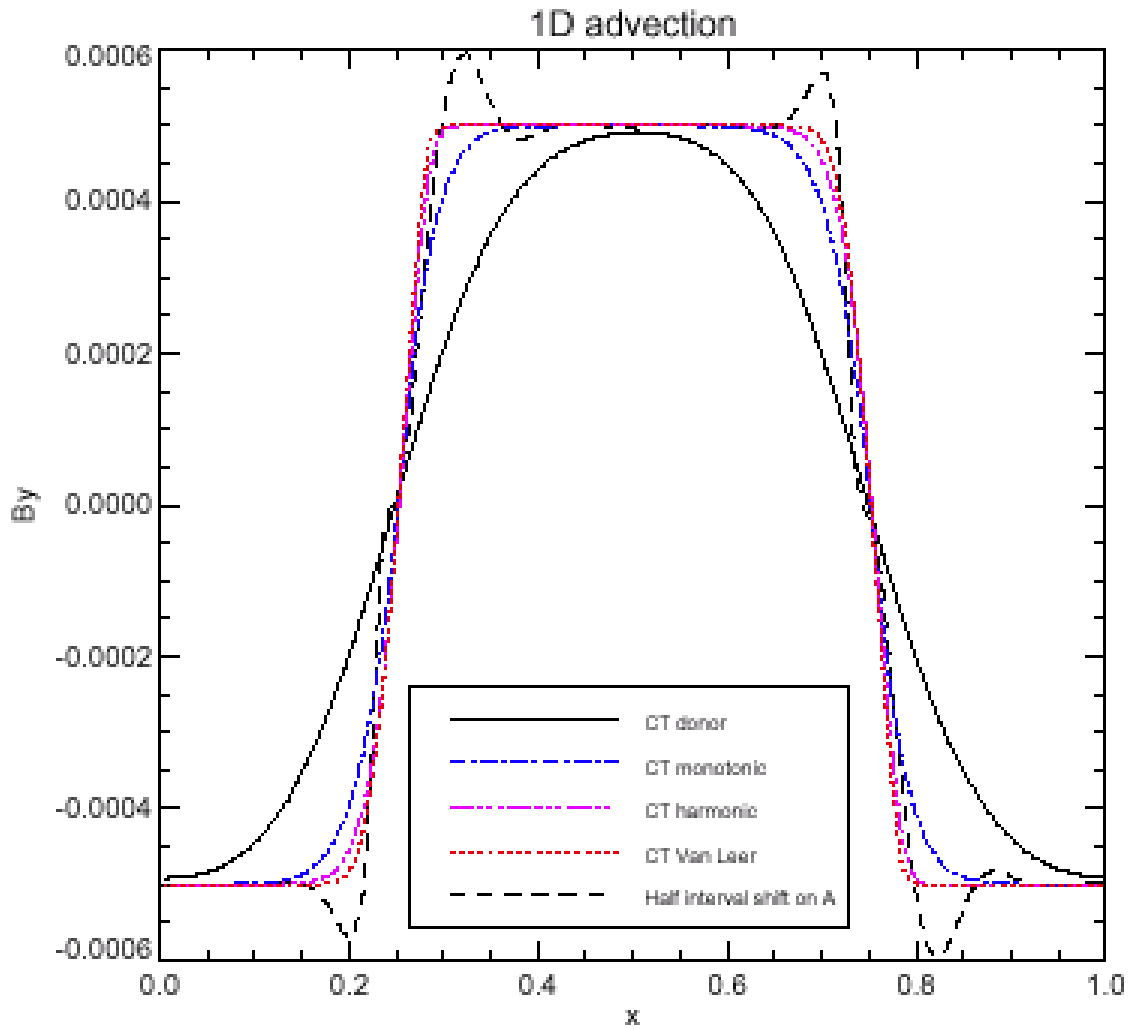
CT 1D advection



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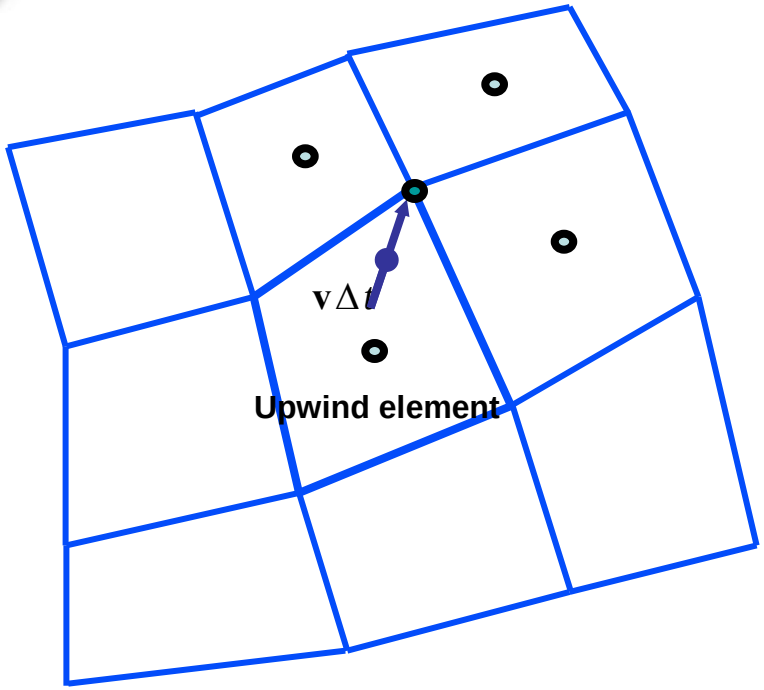
Improved CCT Algorithm



- **Compute B at nodes from the face element representation at element centers. This must be second order accurate. Patch recovery (PR) suggested. Other means are possible.**
- **Compute trial cross face element flux coefficients on each face using these nodal B.**
- **Limit on each face to obtain cross face flux coefficients which contribute zero total flux.**
- **Compute the edge flux contributions in the upwind element by a midpoint integration rule at the center of the edge centered motion vector.**
- **3D coding recently been implemented and is at the verification stage.**

NOTE: All CT algorithms will not conserve magnetic energy. This has consequences for shocks.

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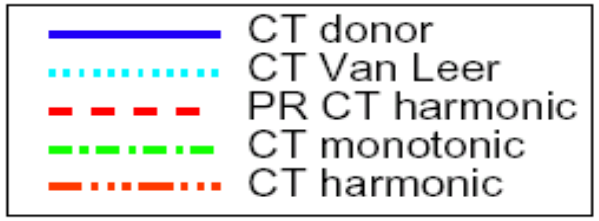
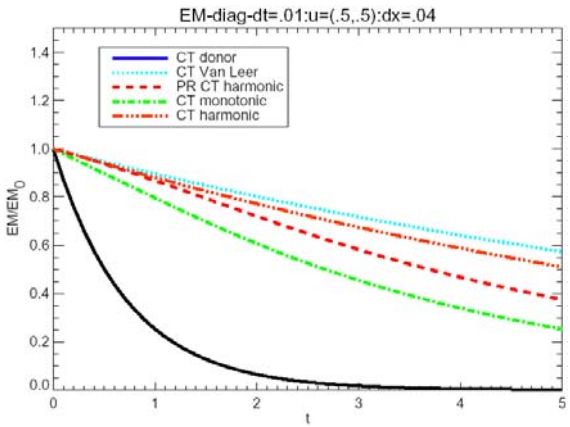
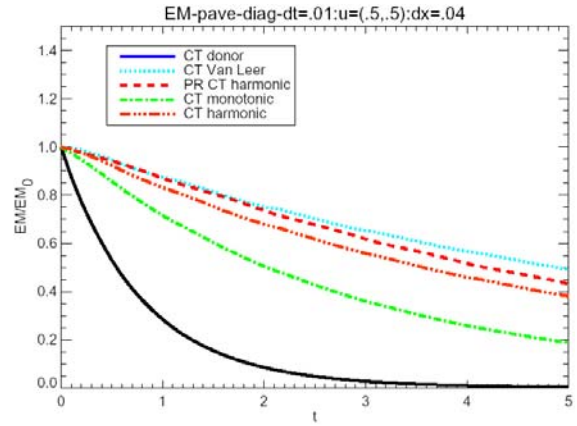
Patch Recovery Based CCT

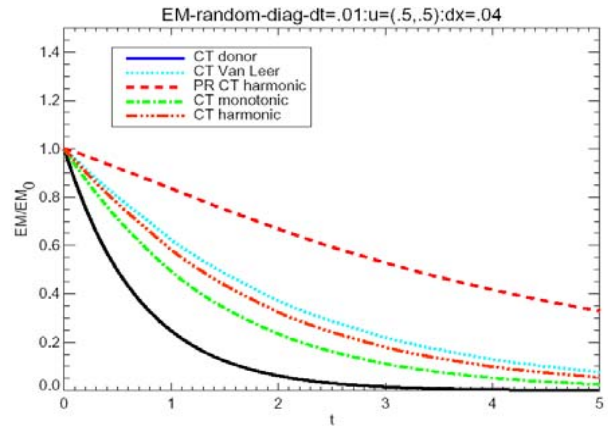


Cartesian | **Paved** | **Randomized**

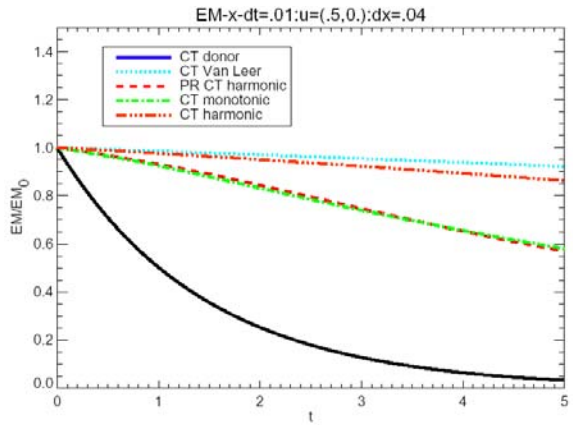
diag

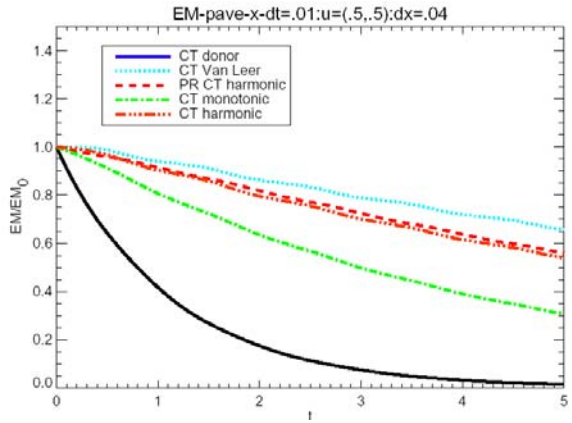


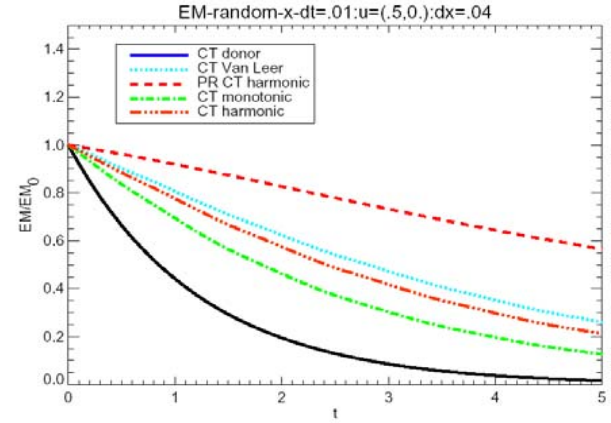




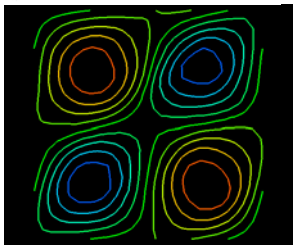
x

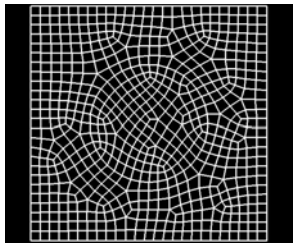


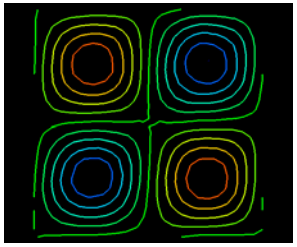




Paved,diagonal, face based, harmonic







Paved,diagonal, patch recovery, harmonic

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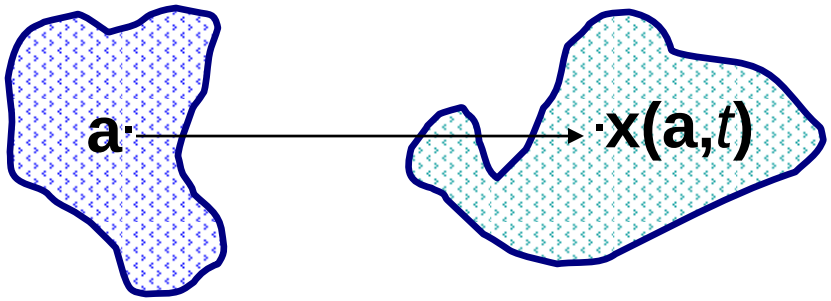
Basic Solid Kinematics



(Reference) Material Coordinates

$$\mathbf{x}(\mathbf{a},t)$$

(Current) Spatial Coordinates

Deformation gradient and inverse:

$$\mathbf{F} = \partial\mathbf{x} / \partial\mathbf{a}$$

$$\mathbf{G} = \mathbf{F}^{-1} = \partial\mathbf{a} / \partial\mathbf{x}$$

Polar Decomposition: **F = VR**

Symmetric Positive Definite (Stretch) Tensor

Proper Orthogonal (Rotation) Tensor

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Remap

- Some material models require that the kinematic description (i.e. F) be available.
- Any method for tracking F on a remapped grid may fail eventually.
  - Det(F)>0
  - Positive definiteness of the stretch, V, can be lost.
  - R proper orthogonal: $RR^T = I$, Det(R)>0.
  - Rows of the inverse deformation tensor $G=F^{-1}$ should be gradients.
- These constraints may not hold due to truncation errors in the remap step and finite accuracy discretizations.
- What is the best approach?
  - "fixes" will be required.
  - Storage, accuracy and speed should be considered.

ALEGRA Solutions

- ALEGRA currently uses an integration scheme to update V and R in the Lagrangian step.
  - Conservatively remap components of both V and R (VR)
  - Conservatively remap components of V and quaternion parameters representing R (QVR)
- We have investigated a constrained transport remap to stay in a curl free space (as opposed to div free) (DG)
- Apply appropriate fixes or projections where possible and necessary.

The stretch can fail to be positive definite after remap (VR/QVR)

Limiting minimum and maximum stretches enables robustness.

Spectral Decomposition

$$\mathbf{V}\mathbf{Q} = \mathbf{Q}\Lambda$$

Eigenvector Rows

Eigenvalue Diagonals.

$$\hat{\lambda}_k = \min(\max(\lambda_k, \lambda_s), 1/\lambda_s)$$

$$\hat{\mathbf{V}} = \mathbf{Q}\hat{\Lambda}\mathbf{Q}^T$$

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Project R to rotation after remap

2D
(VR)

$$\begin{aligned}
\hat{R}_{11} &= (R_{11} + R_{22})/a \\
\hat{R}_{21} &= (R_{21} - R_{12})/a \\
\hat{R}_{12} &= (R_{12} - R_{21})/a \\
\hat{R}_{22} &= (R_{11} + R_{22})/a
\end{aligned}$$

$$a = \sqrt{(R_{11} + R_{22})^2 + (R_{21} - R_{12})^2}$$

3D
(VR)

$$\mathbf{R}^0 = \sqrt{\frac{3}{tr(\mathbf{R}^T\mathbf{R})}}\mathbf{R}.$$

$$\mathbf{R}^{m+1} = \frac{1}{2}\mathbf{R}^m[3\mathbf{I} - (\mathbf{R}^m)^T\mathbf{R}^m]$$

QVR

$$q = q_r / \sqrt{q_r \bar{q}_r}.$$

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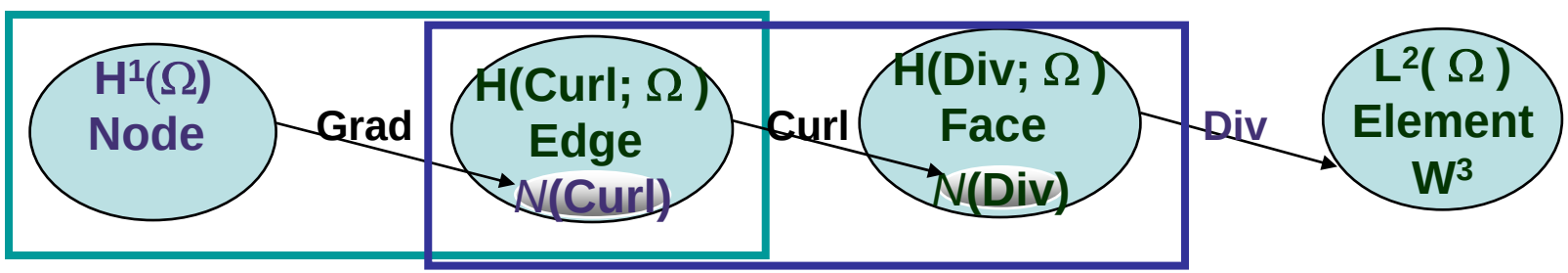
Curl Free Constrained Transport (DG)

- Representation of G on edges allows for a discrete curl-free inverse deformation gradient.
- Remap algorithm should preserve this property.
- Constrained transport (CT) developed by Evans and Hawley for div free MHD algorithm on Cartesian grid is the prototype algorithm.



3-D Solid Kinematics 3-D MHD

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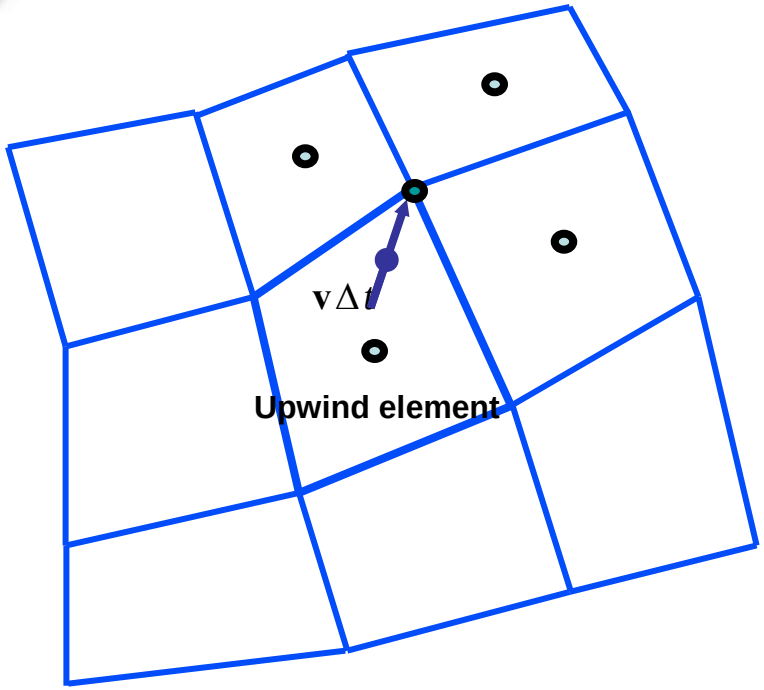
Curl Free Remap Algorithm



Rows guaranteed to be curl free. ☺
No control on det(G). ☹

- **Edge element representation**

$$\mathbf{g}(\xi_1,\xi_2,\xi_3) = \sum_{i\neq j\neq k,\alpha,\beta} \Gamma_{ij}^{\alpha\beta}(\xi_k)\hat{W}_{ij}^{\alpha\beta}$$

- **Use patch recovered nodal values of G to compute trial edge element gradient coefficients along each edge.**

$$\Gamma_{ij}^{\alpha\beta}(\xi_k) = \bar{\Gamma}_{ij}^{\alpha\beta} + s_{ij}^{\alpha\beta}\xi_k$$

- **Limit slopes along each edge (minmod,harmonic)**
- **Compute the node circulation contributions in the upwind element by a midpoint integration rule at the center of the node motion vector.**

$$\int_\Gamma \mathbf{g}\cdot d\mathbf{s} \approx \sum_{i\neq j\neq k,\alpha,\beta} \Gamma_{ij}^{\alpha\beta}(\hat{\xi}_k)(1+\alpha\hat{\xi}_i)(1+\beta\hat{\xi}_j)\delta\xi_k/8$$

- **Take gradient and add to edge element circulations.**

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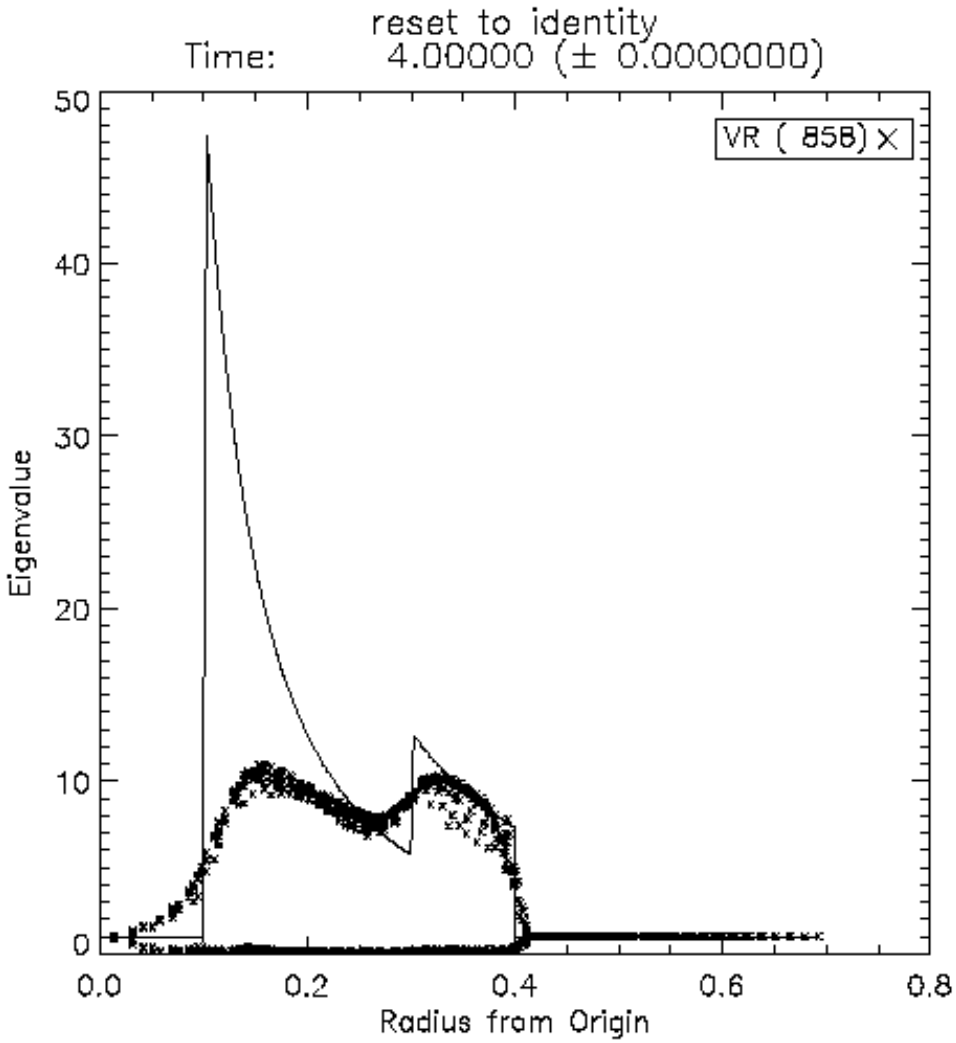
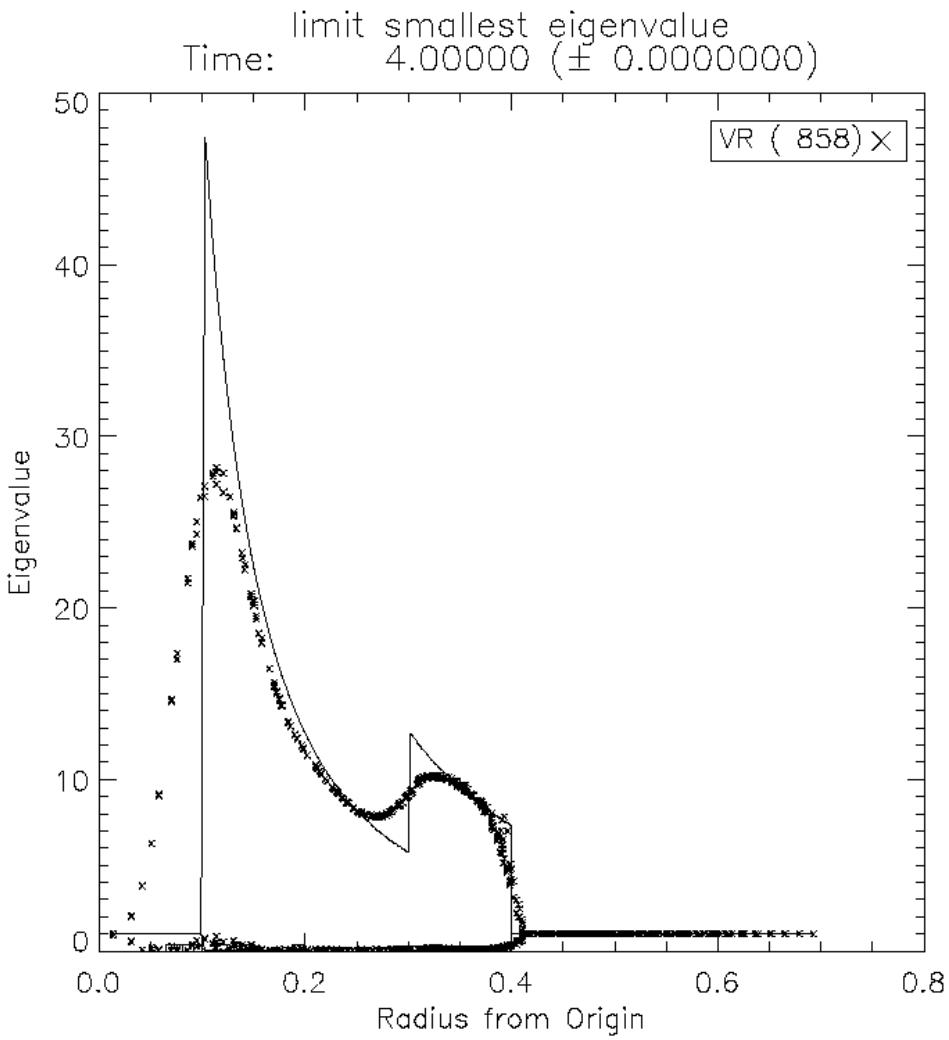
Results for stretch limiter (with small eigenvalue limiting only) (VR/QVR)





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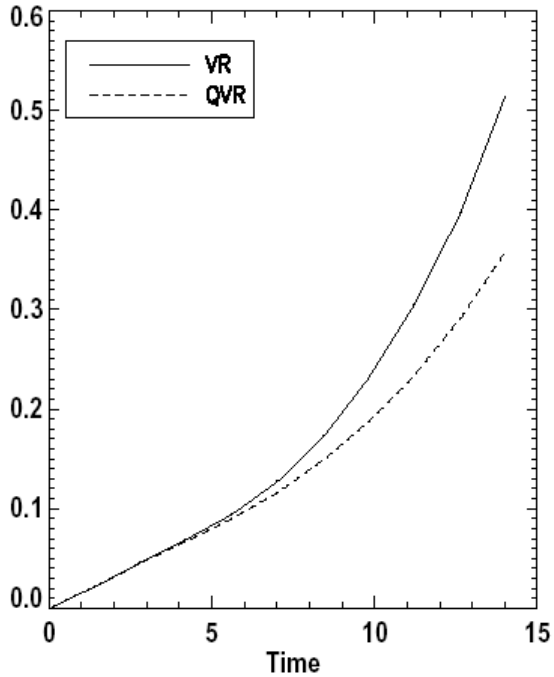
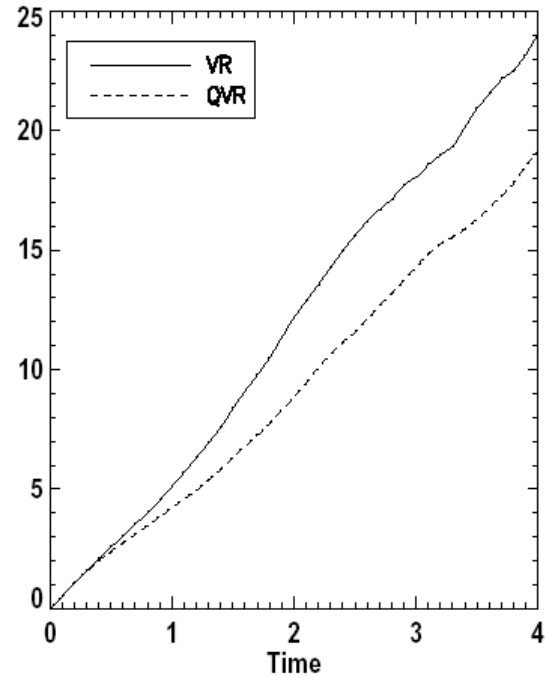
Comparison of 2D ALE Rotation Algorithms for Two Test Problems

Exponential Vortex

$$\mathbf{v}_\theta = \frac{\Gamma}{2\pi r}(1 - e^{-r^2/2})$$



ABC Rotate



$$\mathbf{v}_\theta = \omega_0 r \;\; 0 < r < a$$

$$\mathbf{v}_\theta = \frac{\omega_0 a^2}{r} \;\; a < r < b$$

$$\mathbf{v}_\theta = \frac{\omega_0 a^2}{r}\left(\frac{c^2 - r^2}{c^2 - b^2}\right) \;\; b < r < c$$

$$\mathbf{v}_\theta = 0 \;\; c < r$$

Relative error growth for test problems comparing quaternion with exponential map algorithm (QVR) versus rotation tensor with Cayley transformation (VR)

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Solid kinematics Remap Summary

- Clear significant benefits for using quaternion rotation (LQVR,QVR) representation.
- Stretch tensor reset algorithm based on eigenvalue decomposition has been shown to provide robustness.
- Inverse deformation gradient modeling with curl free remap may warrant continued investigation but must we would need to deal with:
  - Multimaterial
  - Robustness - how to control det(G)
  - Implementation efficiency (Lagrangian and ALE)

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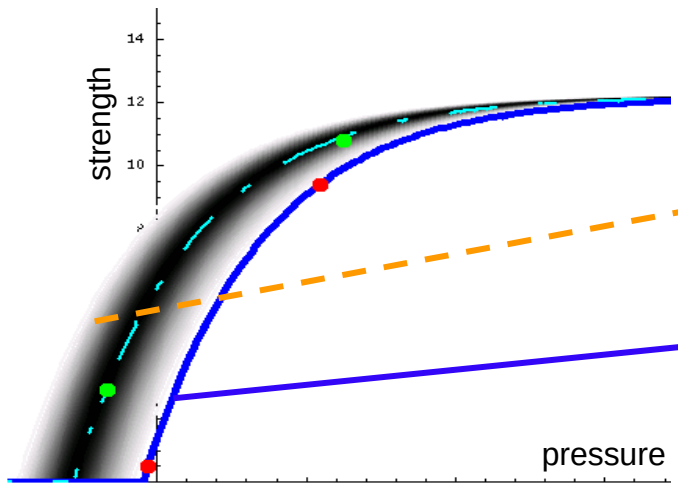
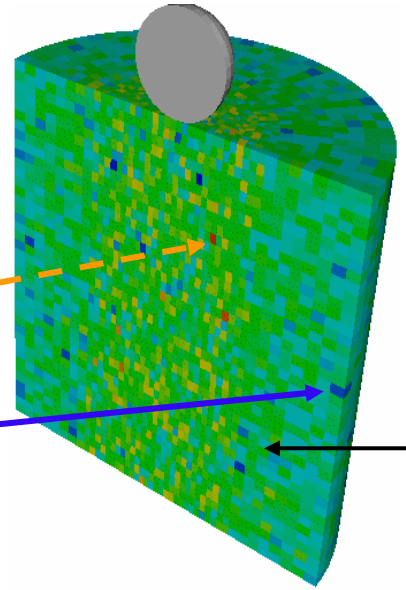
Material Heterogeneity is Integral to Dynamic Failure

Spatially Variable Strength Profile for Ceramics

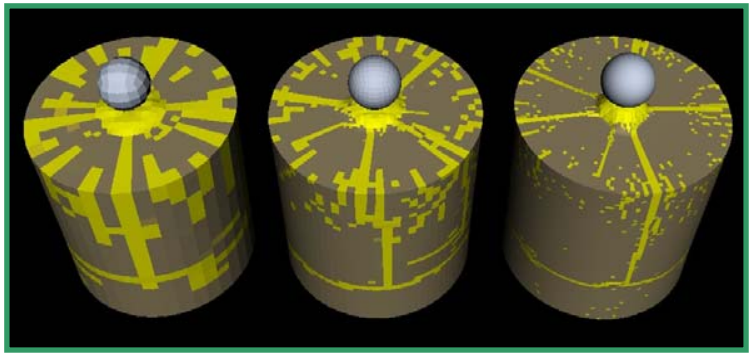




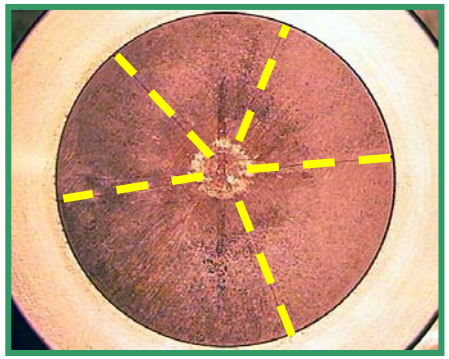
Initial state: small elements are stronger on average, but also more variable

Weibull distribution of strength*:

$$\sigma = \bar{\sigma}\left[\frac{\bar{V}\ln R}{V\ln(1/2)}\right]^{1/m}$$



Reduced Mesh Dependence: Same Model with Uncertainty, Size, and Rate Effects



Comparison to Experiment

Similar crack morphology for different mesh sizes

Formal validation and uncertainty quantification will help identify remaining issues

*Brannon, RM, Wells, JM, and Strack, OE 'Validating Theories for Brittle Damage', Metallurgical and Materials Transactions A, 38A, p. 2861-

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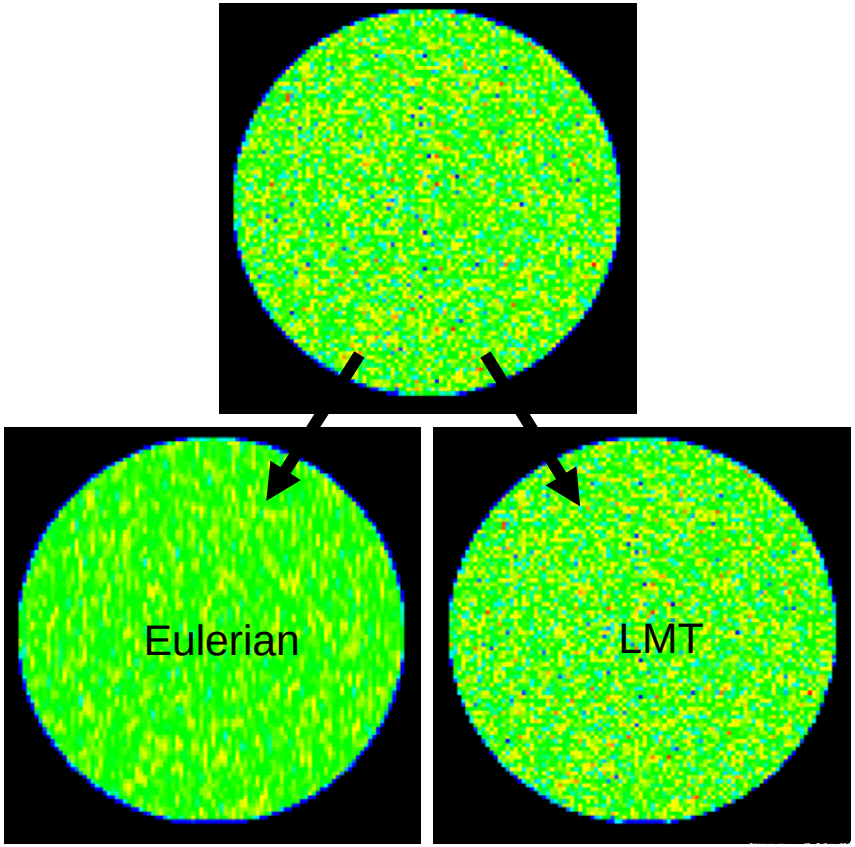
Lagrangian Material Tracking

- **Problem: Need a way to remap highly variable material properties with minimal numerical dissipation.**
- **Idea: Attach properties to material particles.**
- **Erik Strack will discuss work in detail on Wednesday**

Enhancements Needed in ALEGRA to Support Heterogeneity

Initial State



After Remap

Heterogeneous Cylinder Dropping Vertically

Lagrangian Material Tracking (LMT):*

- Standard Eulerian momentum solver (in contrast to other particle methods)
- Variable material properties reside on Lagrangian tracers
- All ALEGRA functionality available
- Transparent to user – no new input/output
- Easily parallelized

* Strack, OE and Hensinger, DM 'The Lagrangian Material Tracer Method for Preserving State Variables in Eulerian Simulations', in preparation

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What about energy conservation with ALE?

We know that we will only get shocks right with ALE if we conserve energy.

Some approach is required to build in total energy conservation. We expect problems with both kinetic energy and magnetic energy.

Our preferred approach here is the so-called DeBar method.

“DeBar fix” for energy conservation

- **We have a modern implementation of DeBar’s kinetic energy treatment.**

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

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

- **It corrects for the process of remap on the kinetic energy and allows full conservation of energy.**
- **We have a switch (Q/p >0.001) to turn the fix off away from shocks.**
- **We can also take care to limit the amount of cooling of a material due to the fix which is used in the Z-pinch implosions, this is NOT the default setting.**
- **Robust/automatic controls are desirable.**

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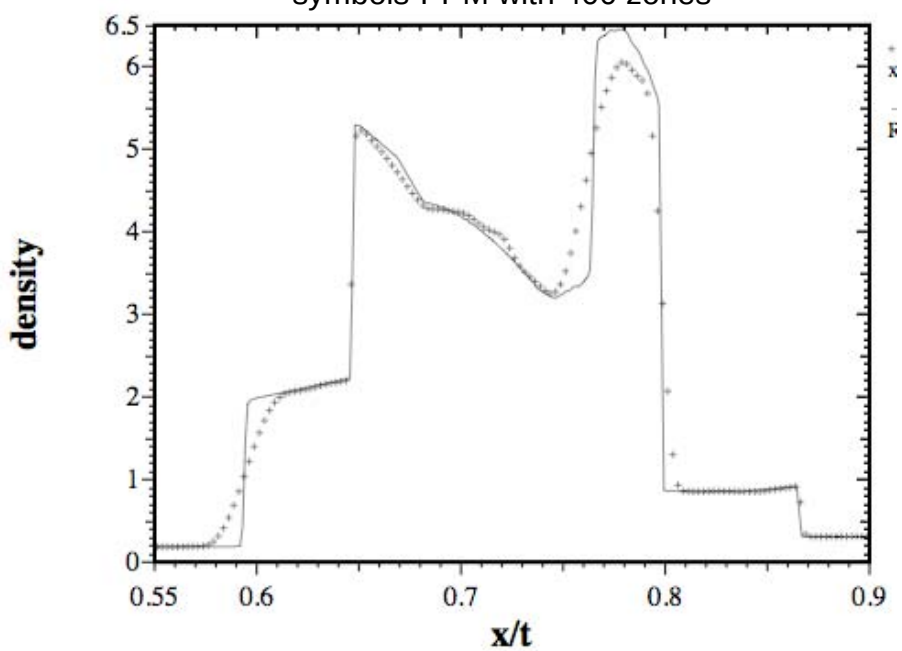
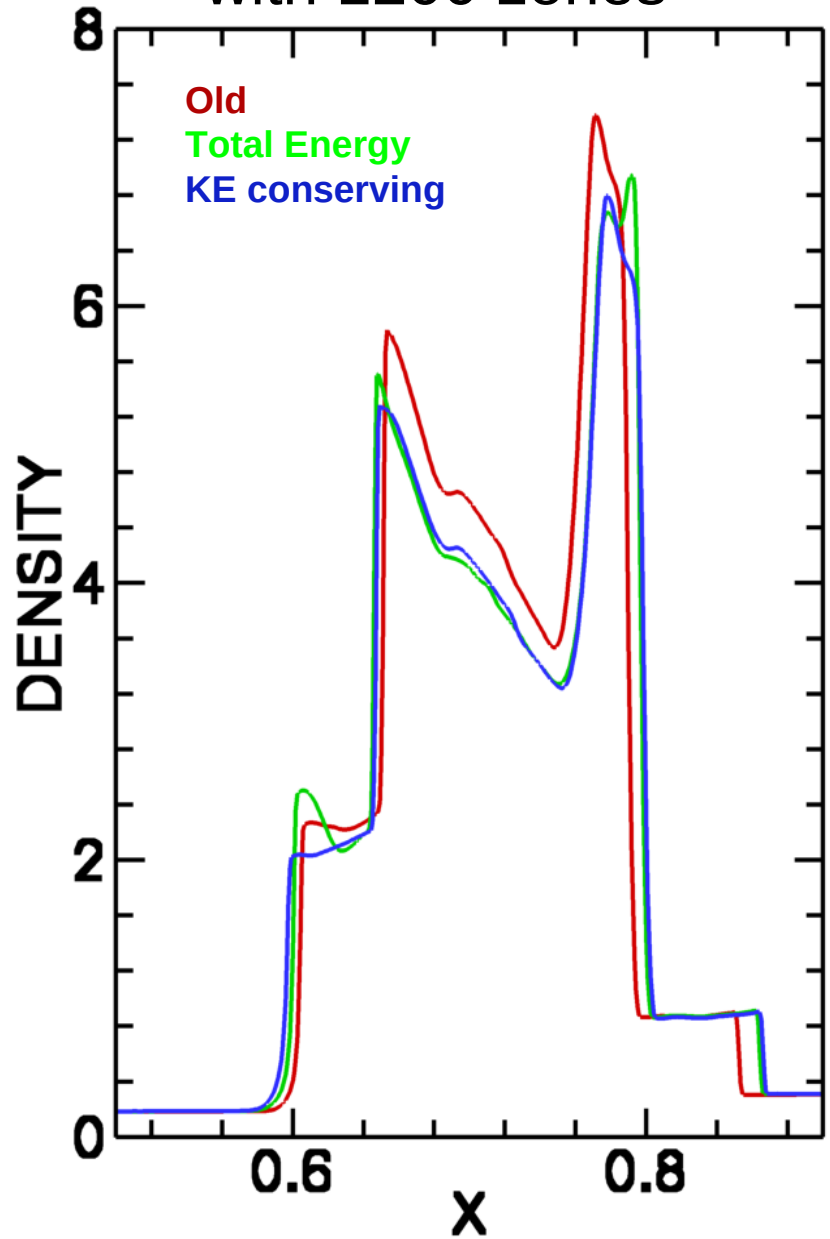
Results with classic Woodward-Colella (W-C) Blast Wave Problem

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

Solid - fiducial 6400 zones
symbols-PPM with 400 zones

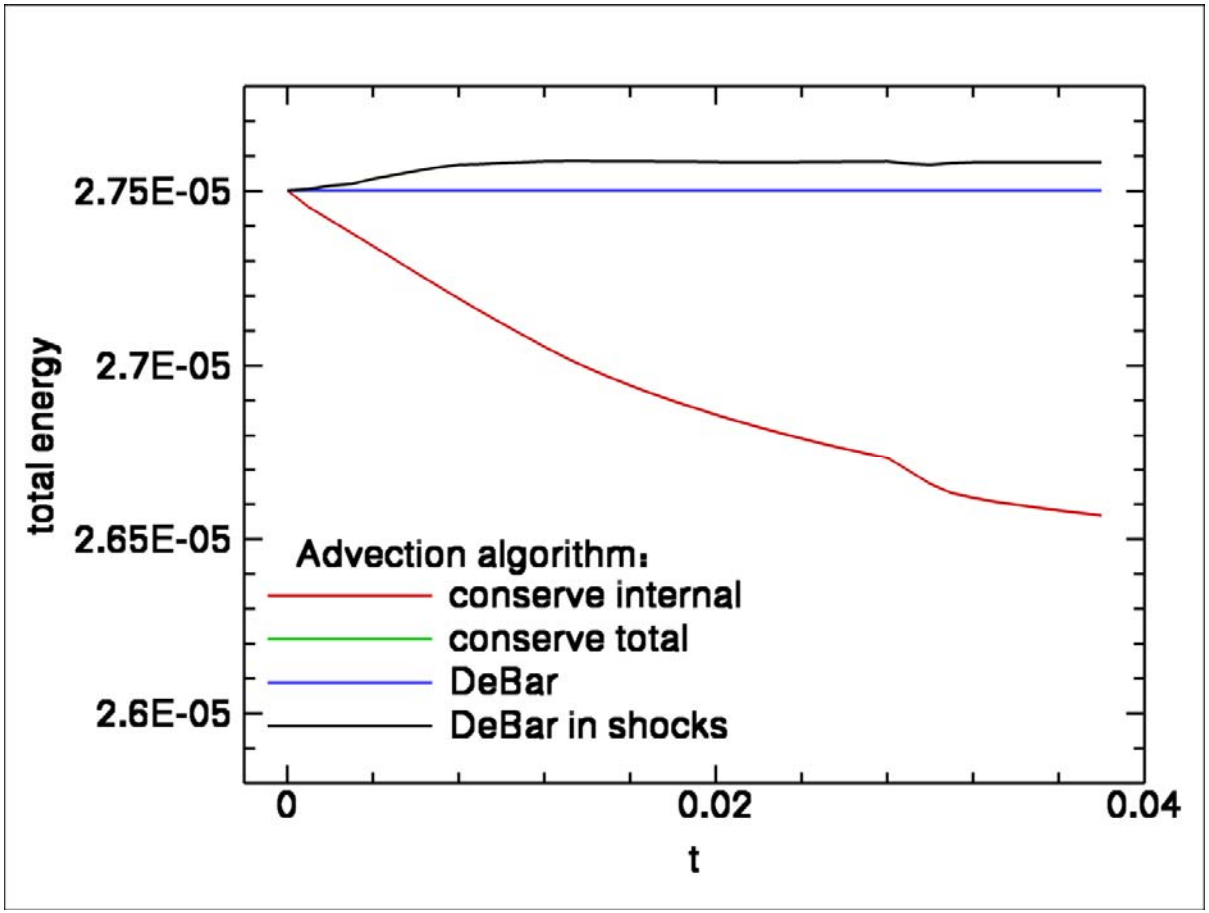


ALEGRA Results
with 1200 zones



Results with W-C Blast Wave Problem (continued)

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



The green curve is hidden by the blue curve.

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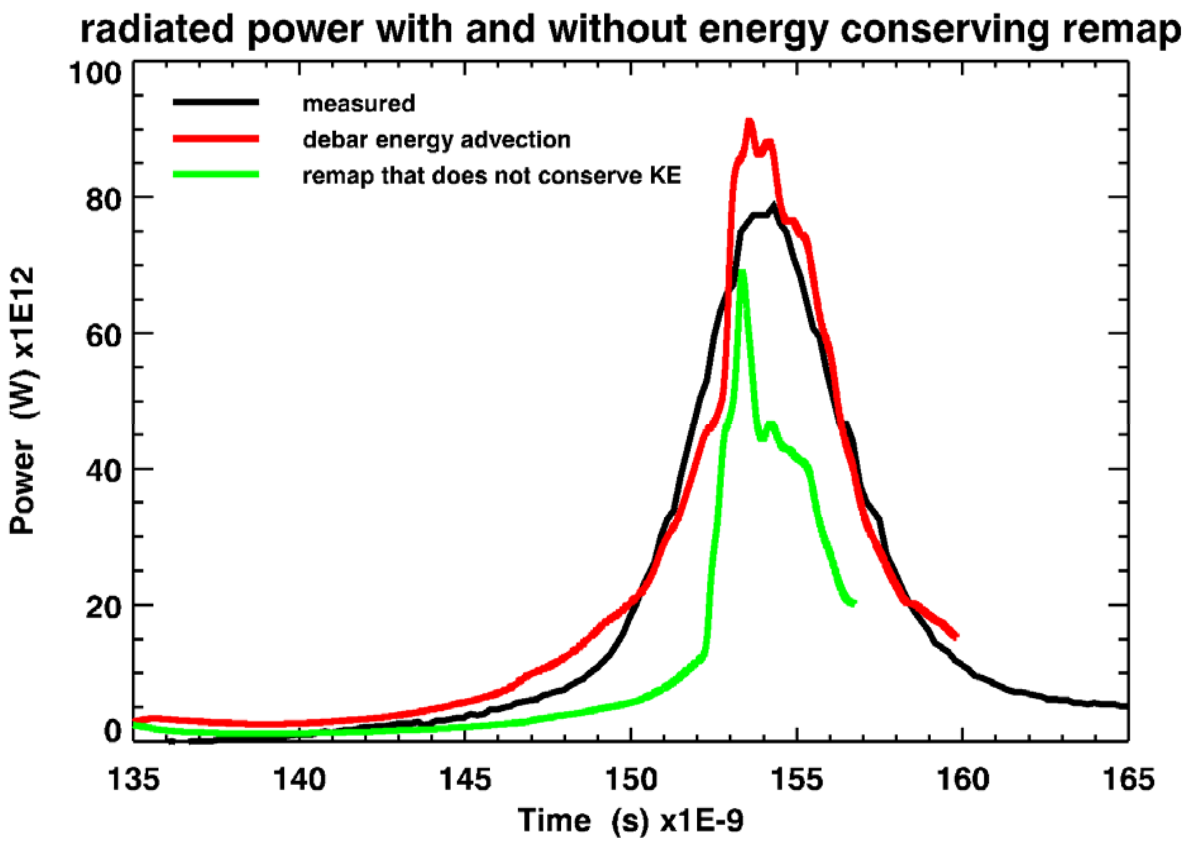
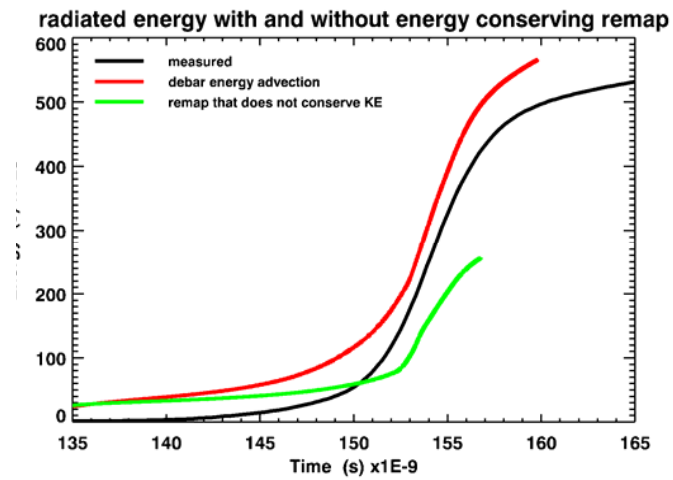
Algorithm Impact: 3D Z-Pinch Implosion

- **This shows the impact of using KE DeBar remap. The radiated power is the key metric. Results are courtesy Ray Lemke.**





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3D DeBar for magnetic energy

- **Implemented in 3D so far.**

$$ME = \int \mathbf{B} \bullet \mathbf{B} / (2\mu) dv$$

$$\rho e = \rho e + ME_{remapped} - \int (\mathbf{B}_{remapped} \bullet \mathbf{B}_{remapped}) / (2\mu) dv$$

- **Implementation uses the same switches/limiters as the KE DeBar**
- **Optional control for KE and/or ME debar**

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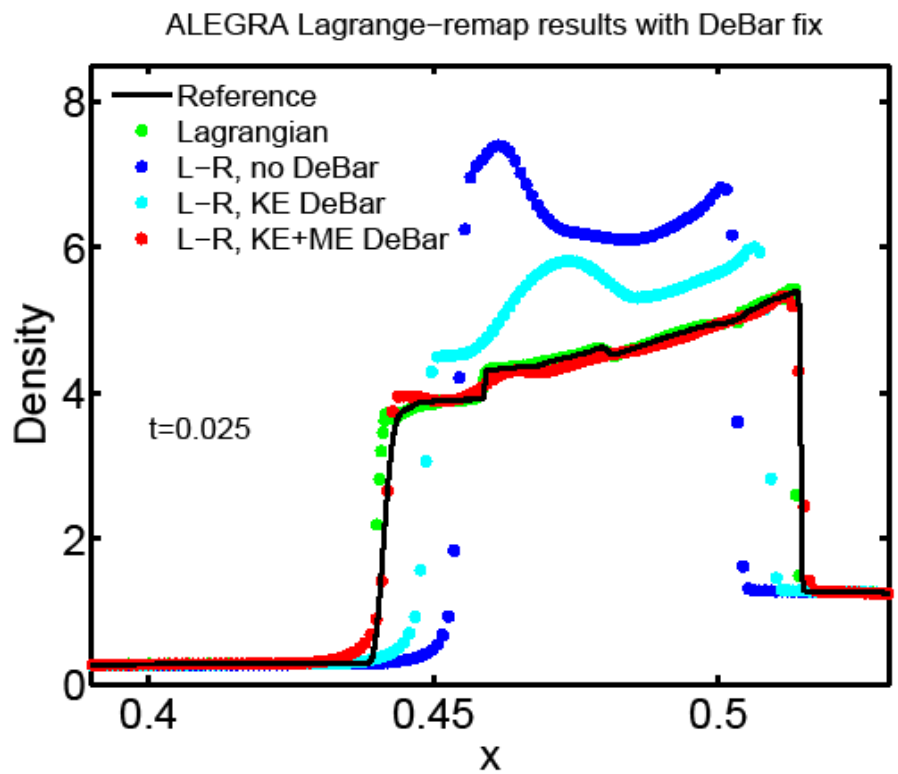
Magnetized Woodward-Colella problem

Uniform **B** field added:

$$\mathbf{B} = 15\hat{x} + 15\hat{y}$$

- Magnetic/kinetic/internal energy densities then have nearly same magnitude

- Failure to conserve magnetic energy exposed in MHD shocks:
  - Shock speeds
  - Post-shock states



- Solution is improved with DeBar correction for KE only
- Solution acceptable only with full DeBar correction (KE + ME)
  - Correct speeds, states and rate of convergence

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Summary

- Lagrange with Eulerian remap is a major operational mode for our users.
- However, simpler and more effective remeshing control is allowing more general remeshing (not just Eulerian) to become more acceptable and useful.
- We are working on improved interface reconstruction and unsplit remap algorithms.
- Constrained transport type remap algorithms can appear in MHD and solid kinematics.
- Robust algorithms to account for discrete kinetic and magnetic energy losses are clearly very important.
- We look forward to continuing improvements across the board in remap methodologies.