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High-order Curvilinear ALE Hydrodynamics

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We are developing high-order ALE discretization methods for large-scale hydrodynamic simulations

The Arbitrary Lagrangian-Eulerian (ALE) framework for the equations of shock hydrodynamics is the foundation of many large-scale simulation codes.

ALE Equations

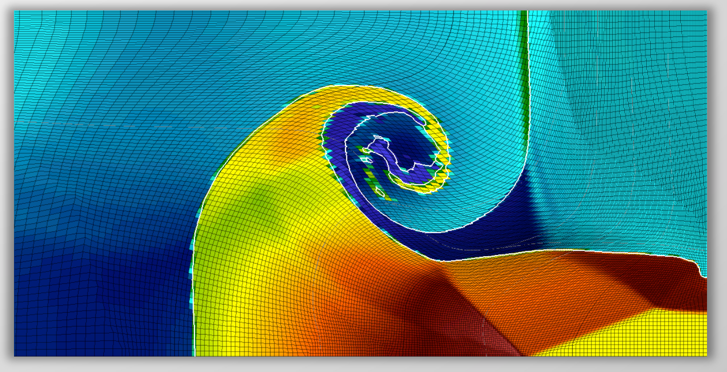
Momentum Conservation: $$\rho\left(\frac{\mathrm{d}\vec{v}}{\mathrm{d}t}+\vec{c}\cdot\nabla\vec{v}\right)=\nabla\cdot\sigma$$

Mass Conservation: $$\frac{\mathrm{d}\rho}{\mathrm{d}t}+\vec{c}\cdot\nabla\rho=-\rho\nabla\cdot\vec{v}$$

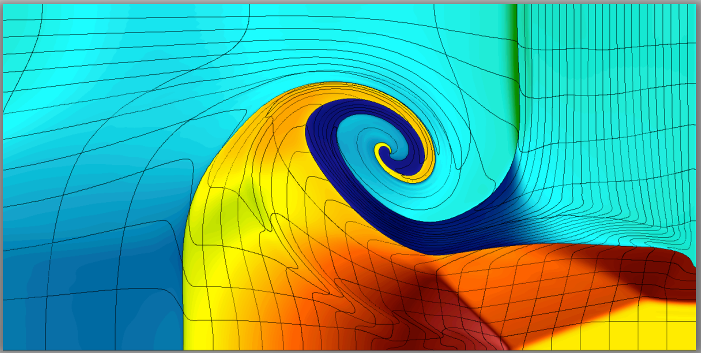
Energy Conservation: $$\rho\left(\frac{\mathrm{d}e}{\mathrm{d}t}+\vec{c}\cdot\nabla e\right)=\sigma:\nabla\vec{v}$$

Equation of State: $$p=EOS(e,\rho)$$

Equation of Motion: $$\frac{\mathrm{d}\vec{x}}{\mathrm{d}t}+\vec{c}=\vec{v}$$



Traditional ALE simulation of a 2D shock triple-point Riemann problem



Purely Lagrangian simulation with high-order Q_8-Q_7 curvilinear finite elements

ALE discretization approaches consist of:

- Lagrange phase
- mesh optimization step
- field remap step
- multi-material zone treatment step

"advection" phase

High-order curvilinear Lagrangian discretizations need a matching accurate "advection" phase

We have developed BLAST - a high-order research Lagrangian hydrocode featuring:

- Curvilinear mesh zones
- High-order kinematic and thermodynamic fields
- Exact conservation on semi-discrete level

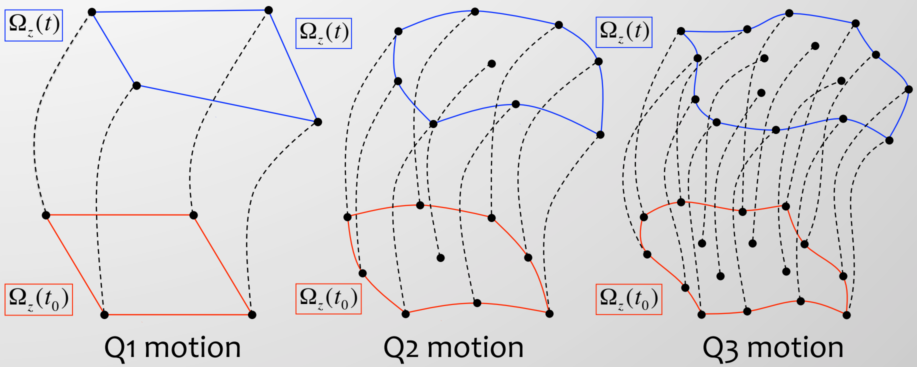
Semi-discrete finite element method

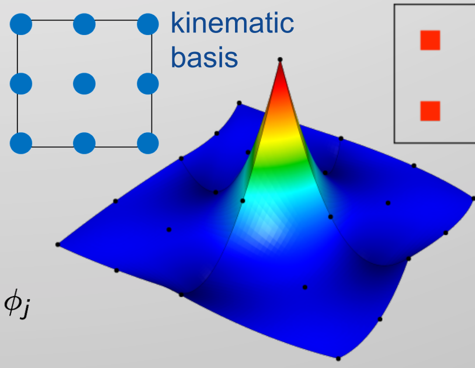
Momentum Conservation: $\mathbf{M_v}\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\mathbf{F}\cdot\mathbf{1}$

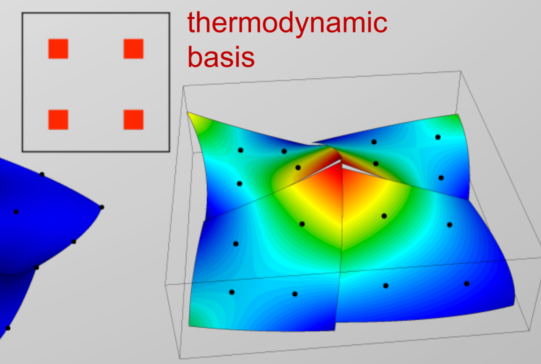
Energy Conservation: $\mathbf{M_e}\frac{\mathrm{d}\mathbf{e}}{\mathrm{d}t} = \mathbf{F}^{\mathbf{T}}\cdot\mathbf{v}$

Equation of Motion: $\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}$

- FLOP-intensive numerical kernel $(\mathbf{F})_{ij} = \int_{\Omega(t)} (\sigma : \nabla \vec{w}_i)\, \phi_j$
- Generalizations of classical SGH schemes

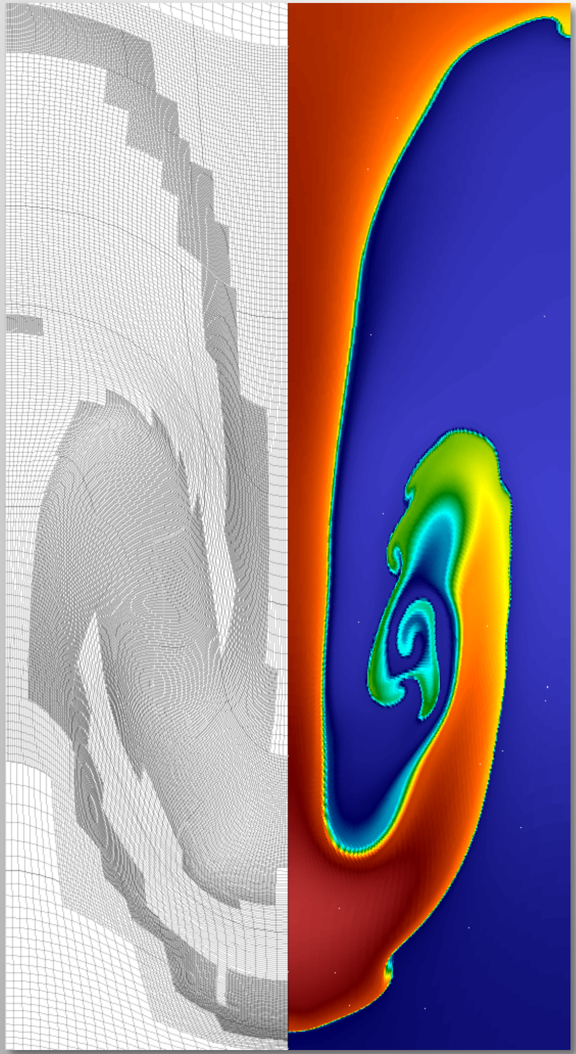




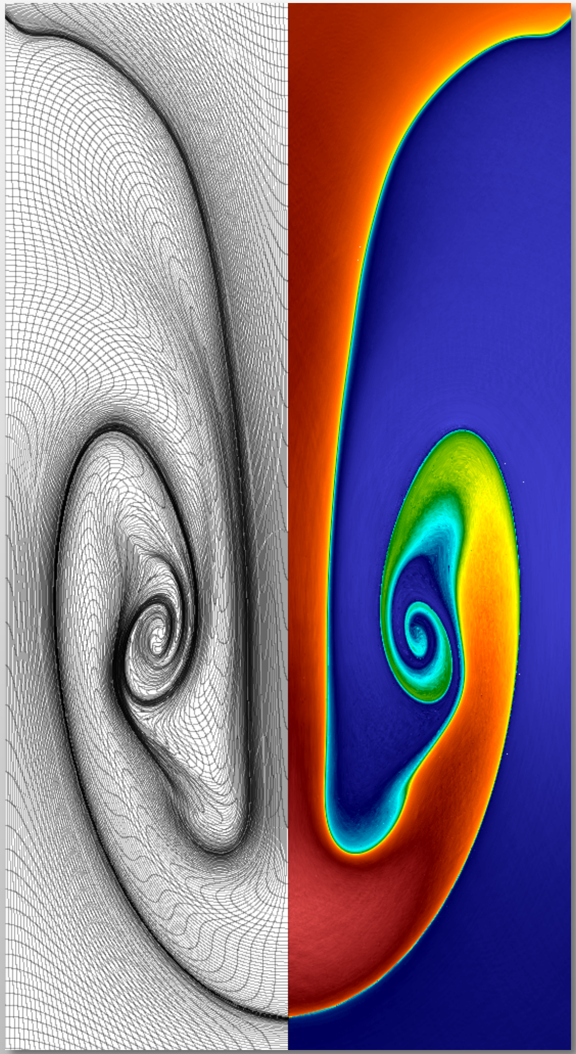


① *Kolev and Rieben*, A Tensor Artificial Viscosity Using a Finite Element Approach, ***JCP*, *2009*.**
② *Dobrev, Ellis, Kolev and Rieben*, Curvilinear finite elements for Lagrangian hydrodynamics, ***IJNMF***, *65(11-12):1295-1310*, ***2010*.**
③ *Dobrev, Kolev and Rieben*, High order curvilinear finite element methods for Lagrangian hydrodynamics, ***SISC*, *2012*.**
④ *Dobrev, Ellis, Kolev and Rieben*, High order curvilinear finite elements for axisymmetric Lagrangian hydrodynamics, ***CAF*, *2012*.**
⑤ *Dobrev, Kolev and Rieben*, High order curvilinear finite elements for elastic-plastic Lagrangian dynamics, ***JCP*, (*submitted*).**
⑥ BLAST: High-order curvilinear finite element code for Lagrangian shock hydrodynamics, http://www.llnl.gov/casc/blast
⑦ MFEM: Parallel finite element discretization library, http://mfem.googlecode.com

High-order Lagrangian simulations can support extreme curvature, but the simulation time-steps become too small



ALE-AMR simulation of RT instability



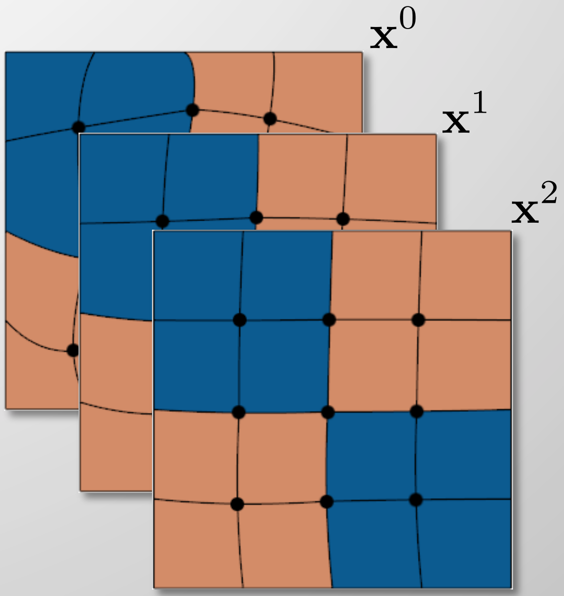
High-order Lagrangian simulation in BLAST

Close-up of the Q_8 curvilinear zones

Prior work related to curvilinear mesh optimization and high-order field remap

- There has been much work on mesh relaxation in the context of low-order meshes (i.e. Q_1 meshes with straight edges), including:
  - Equipotential rezoning (*Winslow, Crowley*)
  - Reference Jacobian based smoothing (*Margolin, Knupp, Shashkov*)
  - Mesquite library: www.cs.sandia.gov/optimization/knupp/Mesquite.html
- There has also been a lot of research on conservative and monotonic field remap (mostly in the lower-order case), such as:
  - Cell-centered remap schemes (*Maire, Loubere, Barlow*)
  - Conservative remap via overlays and swept volumes (*Bailey, Shashkov, Kucharik*)
  - Flux corrected transport (*Kuzmin, Turek, Scovazzi*)
  - Optimization based remap (*Bochev, Rizdal, Scovazzi, Shashkov*)
- There are also alternative approaches such as ReALE based on changing the local mesh connectivity (*Loubere, Maire, Shashkov, Breil, Galera*).
- We want to extend these ideas to the general high-order case.

Harmonic curvilinear mesh optimization



- Mesh optimization is needed in ALE to alleviate small time steps, poor approximation and non-physical behavior.
- The goal is to improve the current mesh with respect to a distortion-related quality metric.
- Harmonic-type mesh relaxation is based on *local averaging* of high order mesh nodes.
- General form: $\boxed{\mathbf{x}^{n+1} = \mathbf{x}^n + M^{-1}(f - L\mathbf{x}^n)}$

  where L is a "high-order mesh Laplacian" and M is a smoother/preconditioner for L.
- The mesh Laplacian is a topological, zero row sum matrix that specify the averaging stencil and weights through its off-diagonal entries.
- For a uniform Q_1 mesh with equal weights, L is a just the scaled 5/7-point Laplacian.
- The relaxation converges to the L - harmonic extension of the boundary nodes to the interior, but the smoother M influences the path to convergence. Other factors: number of iterations, using PCG instead of simple iteration, FEM basis (Bernstein).

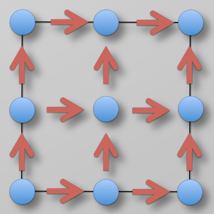
High-order mesh Laplacians and smoothers

There are different approaches to define topological mesh Laplacians for high-order meshes:

1. Use FEM sparsity to connect the high-order nodes with equal weights
   — This doesn't take into account the the differences between element-, face-, edge- and vertex-associated high-order nodes
2. Assemble high-order stiffness matrix by ignoring the transformation to the reference element
   — Mapping to the reference element and its Jacobian: $\Phi_E : \widehat{E} \to E,\ \Phi_E(\hat{x}) = \sum_i \mathbf{x}_{E,i}\hat{\varphi}_k(\hat{i}),\ J_E(\hat{x}) = \nabla\Phi_E(\hat{x}).$
   — Local stiffness matrix, and mesh Laplacian based on its purely topological version:

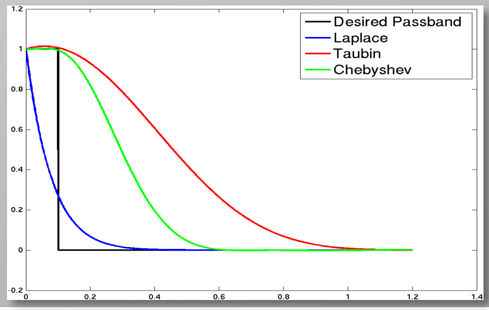
$$(S_E)_{ij} = \int_{\widehat{E}} J_E^{-1}\nabla\hat{\varphi}_i \cdot J_E^{-1}\nabla\hat{\varphi}_j |J_E| \quad \mapsto \quad \mathbf{x}^T \boldsymbol{L_2}\mathbf{x} = \sum_E \mathbf{x}_E^T \widehat{S}\mathbf{x}_E^T = \sum_E \int_{\widehat{E}} \nabla\Phi_E : \nabla\Phi_E$$

3. Use the the "discrete gradient" between the high-order finite element spaces.
   — Let $S_h \subset H^1$ and $V_h \subset H(curl)$ be the high-order nodal and Nedelec FEM spaces.
   — The "discrete gradient" G is the matrix representations of the mapping $\varphi_h \in S_h \mapsto \nabla\varphi_h \in V_h$
   — Note that G is a topological matrix, which is independent of the node coordinates.
   — Globally defined mesh Laplacian: $\boldsymbol{L_3} = \boldsymbol{G}^T\boldsymbol{G}.$

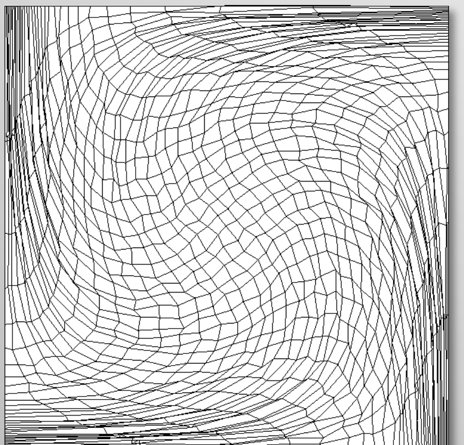


Smoother choices:

1. Diagonal l1-Jacobi
   — Good for symmetry, but slow to converge. From *hypre's* AMS solver
2. Low-frequency preserving polynomial filter
   — *M. Berndt and N. Carlson*, Using Polynomial Filtering for Rezoning in ALE, Multimat '11.

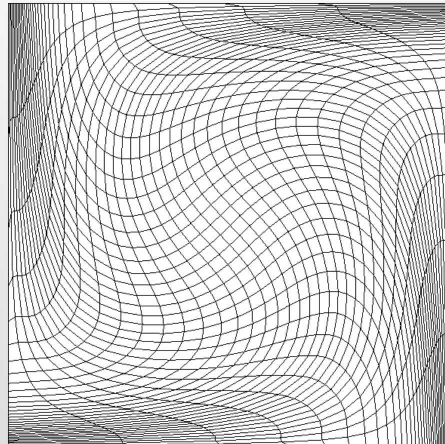


Harmonic relaxation can improve meshes from arbitrary high-order Lagrangian hydro calculations

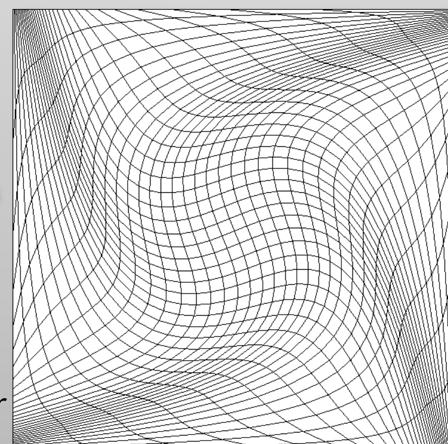


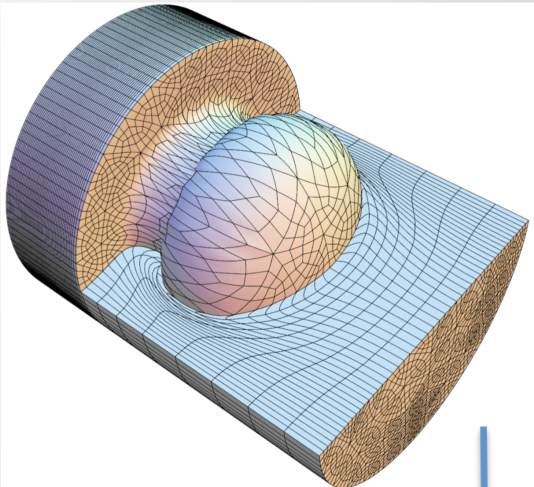
Taylor-Green Q_2 mesh with ``long-wavelength'' and random ``short-wavelength'' perturbation

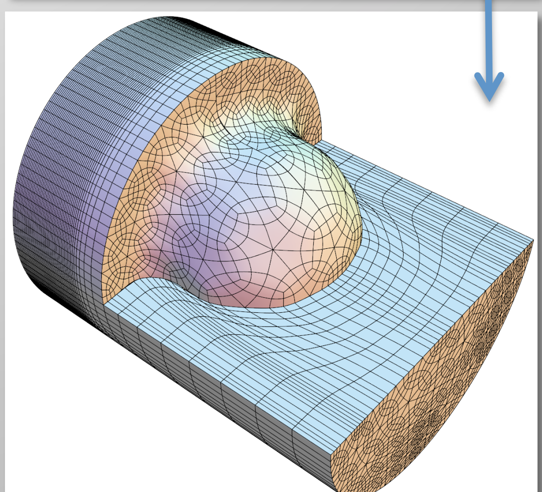
L_3 Laplacian with polynomial smoother (20 iterations)



L_3 Laplacian with diagonal smoother (20 iterations)







Tangential L_2 smoothing of 3D triple-point shock Q_2 mesh (150 iterations).

Inverse-harmonic curvilinear mesh optimization

- Harmonic smoothing is an integral minimization problem:

$$\min_{\mathbf{x}_\mathcal{I}} \left(\frac{1}{2} \mathbf{x}^T L \mathbf{x} \right) = \min_{\mathbf{x}_\mathcal{I}} \left(\frac{1}{2} \sum_E \int_{\widehat{E}} \nabla \Phi_E : \nabla \Phi_E \right) = \min_{\mathbf{x}_\mathcal{I}} \sum_E \int_{\widehat{E}} W(J_E(\hat{x}))\, d\hat{x}$$

where $W(J) \equiv \frac{1}{2}(J : J) = \frac{1}{2} \operatorname{tr}\left(J^T J\right)$. (continuous form of the nodal $\|J\|^2 - 2\det J$)

- The inverse-harmonic (Crowley/Winslow) method minimizes the gradient norm of the inverse maps:

$$\min_{\mathbf{x}_\mathcal{I}} F(\mathbf{x}) \equiv \min_{\mathbf{x}_\mathcal{I}} \left(\frac{1}{2} \sum_E \int_E \nabla(\Phi_E^{-1}) : \nabla(\Phi_E^{-1}) \right) = \min_{\mathbf{x}_\mathcal{I}} \sum_E \int_{\widehat{E}} W(J_E(\hat{x}))\, d\hat{x}$$

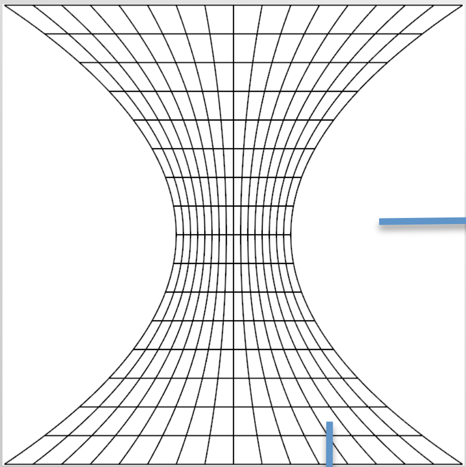
where $W(J) \equiv \frac{1}{2} \det(J) \operatorname{tr}(J^{-T} J^{-1})$. (continuous form of the 2D nodal $\|J\|^2/(2\det J) - 1$)

- General nonlinear smoothing iteration

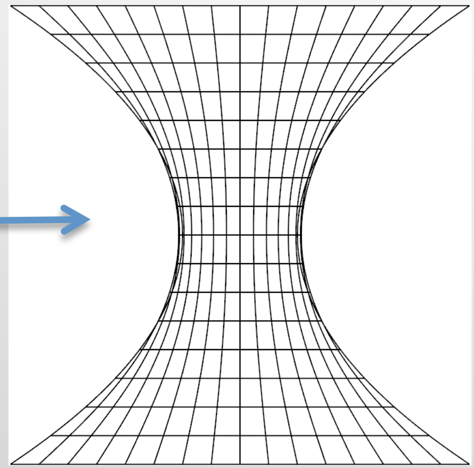
$$\boxed{\mathbf{x}^{n+1} = \mathbf{x}^n - \left[\mathcal{H} F(\mathbf{x}^n)\right]^{-1} \nabla F(\mathbf{x}^n)}$$

- Hessian is inverted with one of the methods used for harmonic smoothing.
- Finite elements enable us to minimize on functional level, i.e. we assemble exactly the functional F, its gradient, etc. element-by-element based on W.
- Other choices for W (e.g. non-linear elasticity) are possible.

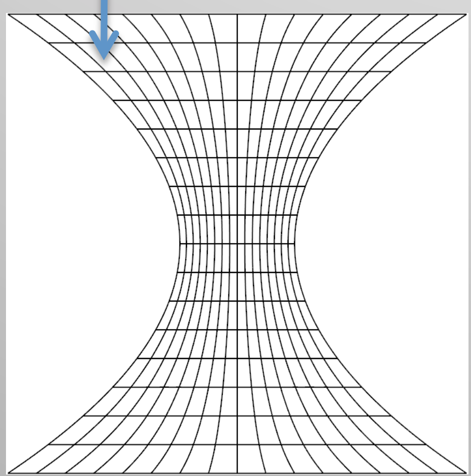
Nonlinear mesh smoothing can provide additional robustness on very deformed grids



Original mesh

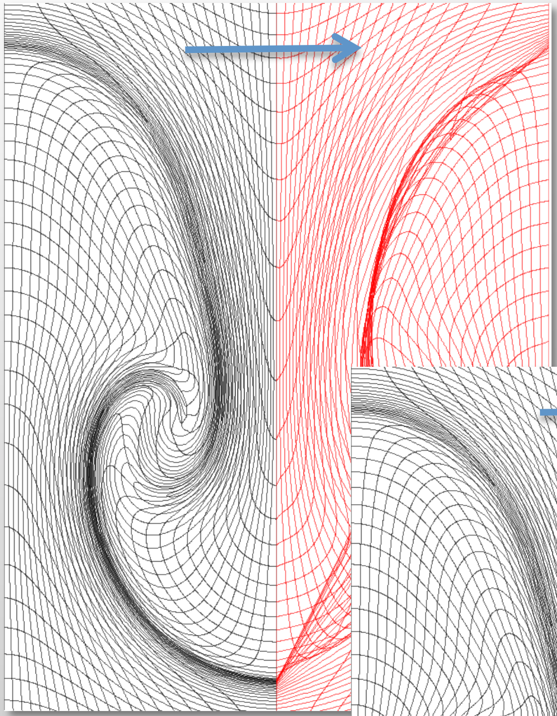


Harmonic smoothing

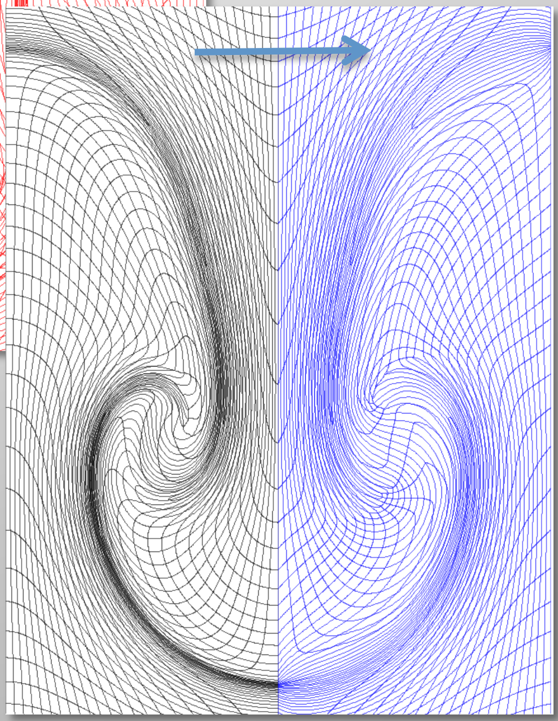


Nonlinear smoothing

Rayleigh-Taylor Q_4 mesh



Harmonic smoothing (L2, 200 iterations)



Nonlinear smoothing (20/200 inner/outer iterations)

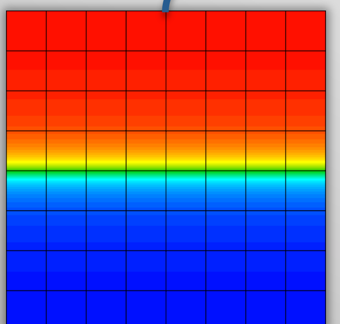
The advection phase can be viewed as a "pseudo-time" extension of the Lagrangian motion

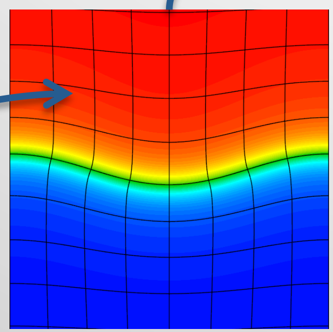
Lagrangian phase

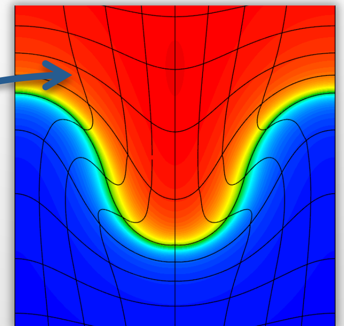
- mesh motion determined by physical velocity
- time t evolution

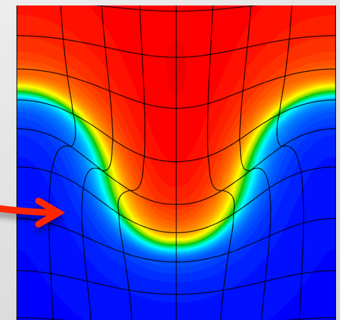
Advection phase

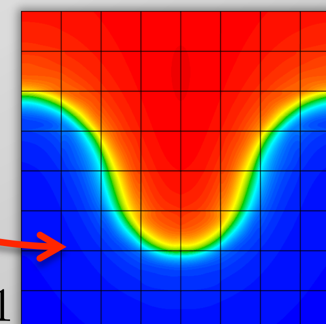
- artificial mesh motion, defining the mesh velocity
- "pseudo-time" τ evolution











Both phases

- ✓ material derivative based on particle trajectories

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} \equiv \frac{\partial \rho}{\partial t} + v_m \cdot \nabla \rho$$

- ✓ Deforming test functions

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} = 0$$

- ✓ Reynolds transport theorem

$$\frac{\partial}{\partial t} \int_{U(t)} \rho = \int_{U(t)} \frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho \nabla \cdot v_m$$

Lagrangian phase ($\vec{c} = \vec{0}$)

Momentum Conservation:	$\rho \frac{\mathrm{d}\vec{v}}{\mathrm{d}t} = \nabla \cdot \sigma$
Mass Conservation:	$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho \nabla \cdot \vec{v}$
Energy Conservation:	$\rho \frac{\mathrm{d}e}{\mathrm{d}t} = \sigma : \nabla \vec{v}$
Equation of Motion:	$\frac{\mathrm{d}\vec{x}}{\mathrm{d}t} = \vec{v}$

Advection phase ($\vec{c} = -\vec{v}_m$)

Momentum Conservation:	$\frac{\mathrm{d}(\rho\vec{v})}{\mathrm{d}\tau} = \vec{v}_m \cdot \nabla(\rho\vec{v})$
Mass Conservation:	$\frac{\mathrm{d}\rho}{\mathrm{d}\tau} = \vec{v}_m \cdot \nabla \rho$
Energy Conservation:	$\frac{\mathrm{d}(\rho e)}{\mathrm{d}\tau} = \vec{v}_m \cdot \nabla(\rho e)$
Mesh velocity:	$\vec{v}_m = \frac{\mathrm{d}\vec{x}}{\mathrm{d}\tau}$

Discontinuous Galerkin weak formulation of pseudo-time advection of discontinuous fields

Element-wise weak formulation of pseudo-time advection based on:
linear motion ($v_m = u$), pseudo-time RTT and deforming test functions

$$\boxed{\frac{d\rho}{d\tau} = u \cdot \nabla \rho}$$

$$\frac{\partial}{\partial \tau} \int_\Omega \rho\psi = \int_\Omega \frac{\mathrm{d}}{\mathrm{d}\tau}(\rho\psi) + \rho\psi \nabla \cdot u = \int_\Omega u \cdot \nabla \rho \psi + \rho\psi \nabla \cdot u = \int_\Omega \nabla \cdot (\rho u)\psi$$

$$= \sum_{T \in \mathcal{T}(\tau)} \int_T \nabla \cdot (\rho u)\psi = - \sum_{T \in \mathcal{T}(\tau)} \int_T \rho u \cdot \nabla \psi + \int_{\partial T} \rho u \cdot n \psi$$

$$= - \sum_{T \in \mathcal{T}(\tau)} \int_T \rho u \cdot \nabla \psi + \sum_{f \in \mathcal{F}_i(\tau)} \int_f \{\rho(u \cdot n_f)\} [\![\psi]\!] + \cancel{\sum_{f \in \mathcal{F}_i(\tau)} \int_f [\![\rho(u \cdot n_f)]\!] \{\psi\}}$$

Discontinuous Galerkin method with Godunov (upwind) flux

$$\frac{\partial}{\partial \tau} \int_\Omega \rho\psi = - \sum_{T \in \mathcal{T}(\tau)} \int_T \rho u \cdot \nabla \psi + \sum_{f \in \mathcal{F}_i(\tau)} \int_f (u \cdot n_f)\{\rho\} [\![\psi]\!] - \frac{1}{2} \sum_{f \in \mathcal{F}_i(\tau)} \int_f |u \cdot n_f| [\![\rho]\!] [\![\psi]\!]$$

Matrix form assuming trial and test function in the same FEM space with mass matrix $\mathbf{M}$:

$$\boxed{\frac{\partial}{\partial \tau}(\mathbf{M}\boldsymbol{\rho}) = \mathbf{A}\boldsymbol{\rho}}$$

Properties: $\mathbf{A}^T \mathbf{1} = 0$

$$\frac{\partial \mathrm{M}}{\partial \tau} = (\mathbf{A} + \mathbf{S}) + (\mathbf{A} + \mathbf{S})^T$$

High-order DG advection algorithms for conservative and accurate remap

moment-based formulation

$$\boxed{\frac{\partial \mathbf{m}}{\partial \tau} = \mathbf{A}\mathbf{M}^{-1}\mathbf{m}} \quad \boldsymbol{m}(\tau) \equiv \int_{\Omega(\tau)} \rho\psi = \mathbf{M}\boldsymbol{\rho} \longrightarrow$$ mass conservation

function-based formulation

$$\boxed{\frac{\partial \boldsymbol{\rho}}{\partial \tau} = -\mathbf{M}^{-1}(\mathbf{A}^{\mathrm{T}} + 2\mathbf{S})\boldsymbol{\rho}} \longrightarrow$$ preservation of constants, linears

- Finite element functions are remapped by integrating the above ODEs in pseudo-time.
- The two approaches are the same on semi-discrete but differ on fully-discrete level.
- Mass conservation + constant preservation can be achieved on fully-discrete level by integrating the mass matrix in pseudo-time.
- A space-time DG method related to these approaches can be viewed as high-order generalization of the classical "swept-volume" method.

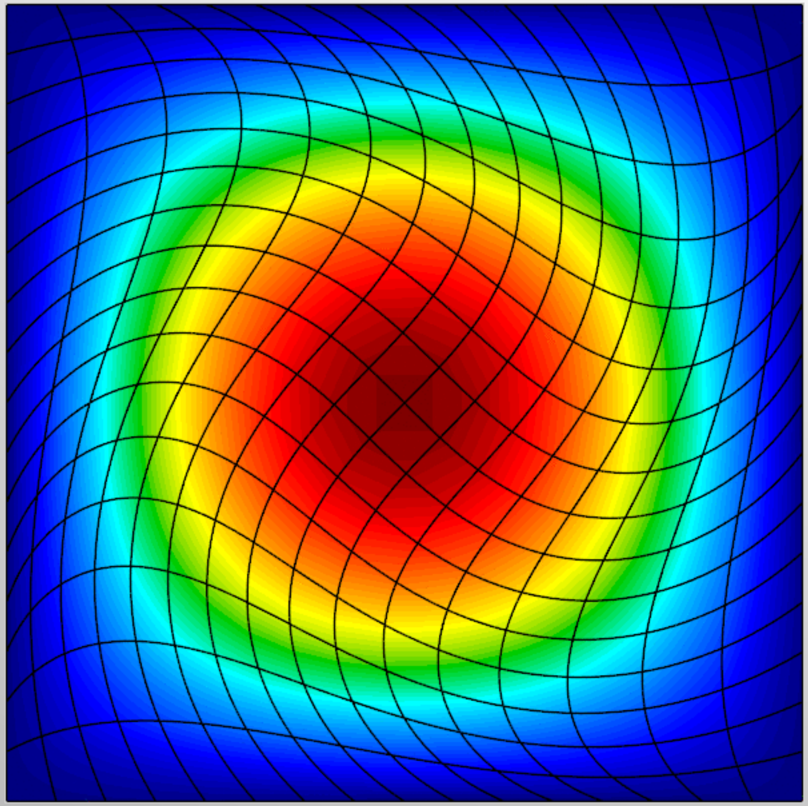
Velocity remap: pseudo-time advection of momentum using continuous FEM space

$$\frac{d(\rho v)}{d\tau} = u \cdot \nabla(\rho v) \quad \mapsto \quad \frac{\partial}{\partial \tau}\int_\Omega \rho(v \cdot w) = -\int_\Omega \rho(u \cdot \nabla w \cdot v) \longrightarrow$$ conservation of momentum

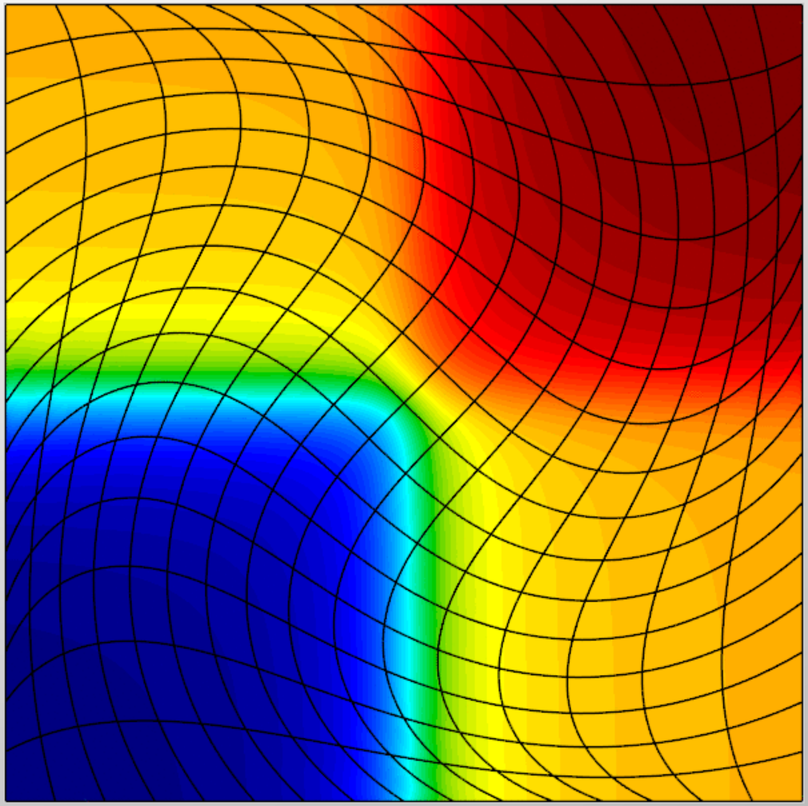
IE remap: pseudo-time advection of density-weighted internal energy using discontinuous FEM

$$\frac{d(\rho e)}{d\tau} = u \cdot \nabla(\rho e) \quad \mapsto \quad \frac{\partial}{\partial \tau}\int_\Omega \rho(e\psi) = -\sum_T \int_T \rho(eu \cdot \nabla\psi) + \sum_f \int_f (u \cdot n_f)\{\rho e\}[\![\psi]\!] - \frac{1}{2}|u \cdot n_f|[\![\rho e]\!][\![\psi]\!]$$

Remap of prescribed smooth fields on smoothly distorted grid (parallel implementation with V.Tomov, TAMU)



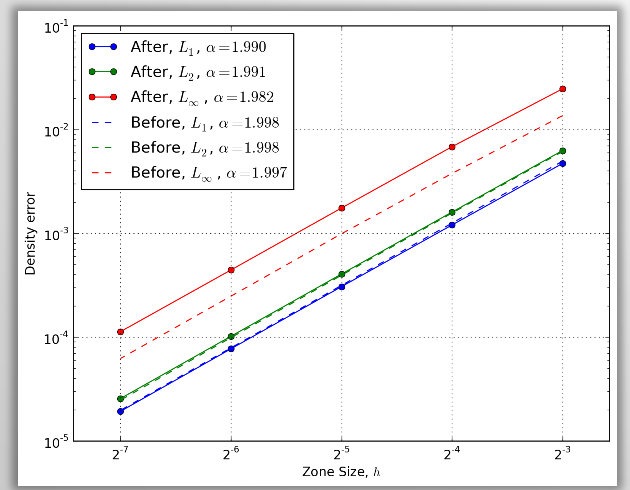
density

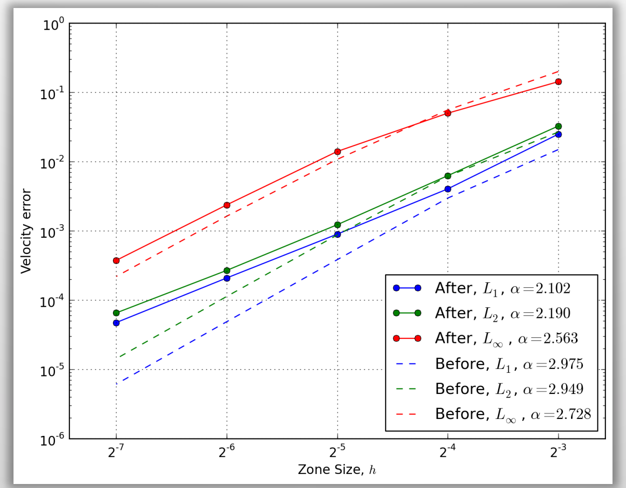


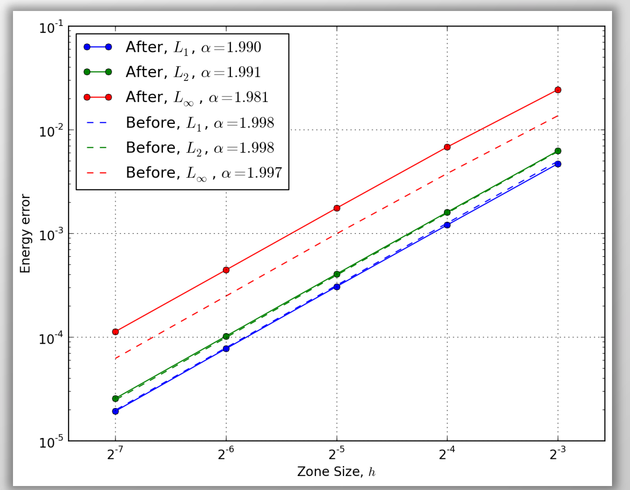
speed

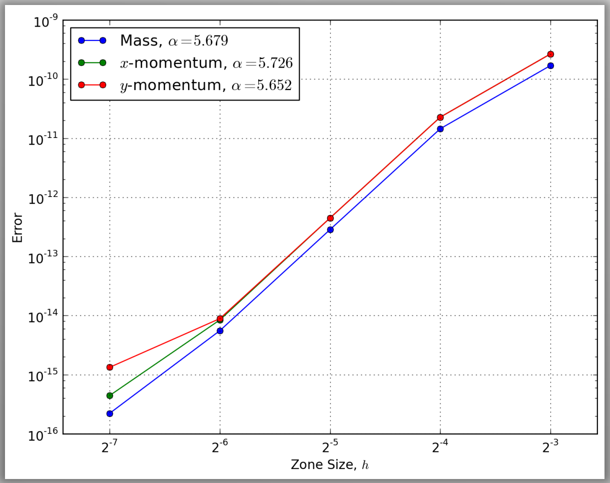
- Q_2-Q_1 method, full mesh relaxation (100 iterations), 20 RK4 steps
- prescribed smooth mesh distortion, $$\rho = e = 1.5 + \sin \pi x \sin \pi y$$ $$v_{\{x,y\}} = \pi/2 + \arctan(20(\{x,y\} - 0.5))$$

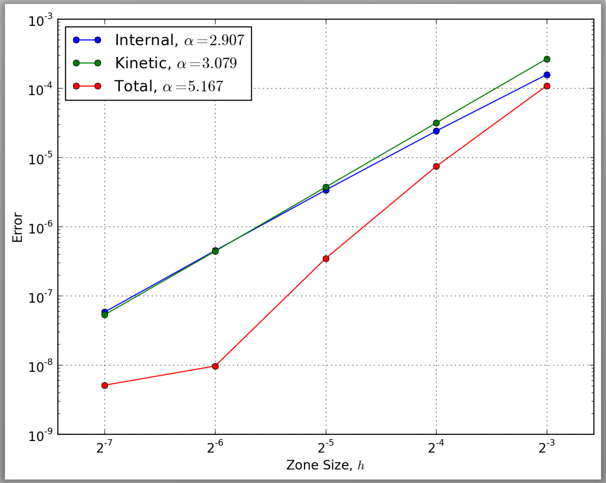
Convergence and errors for the remap of prescribed smooth fields on smoothly distorted grid with Q_2-Q_1 spaces





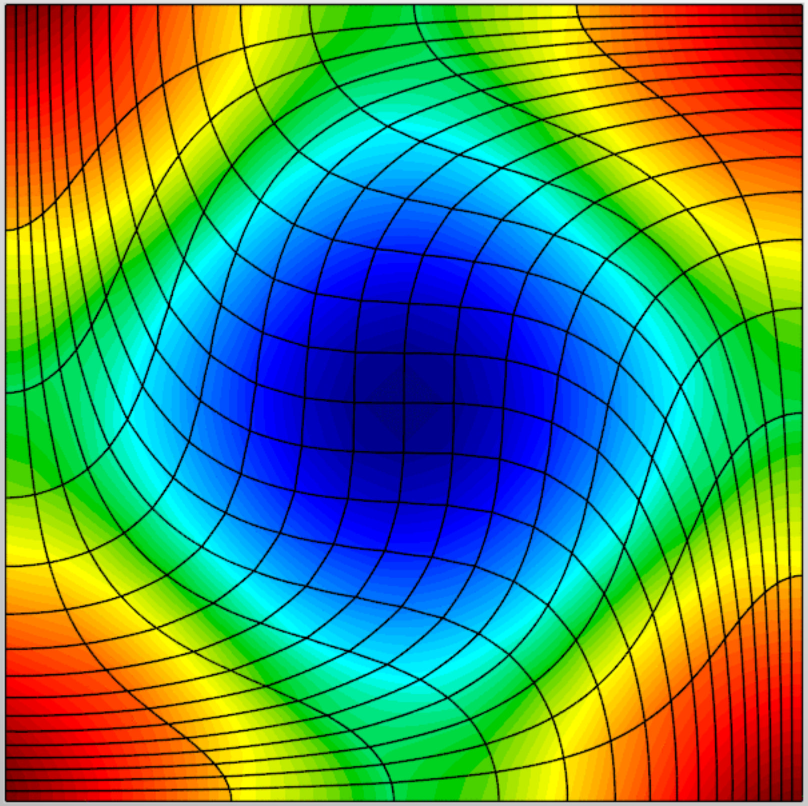




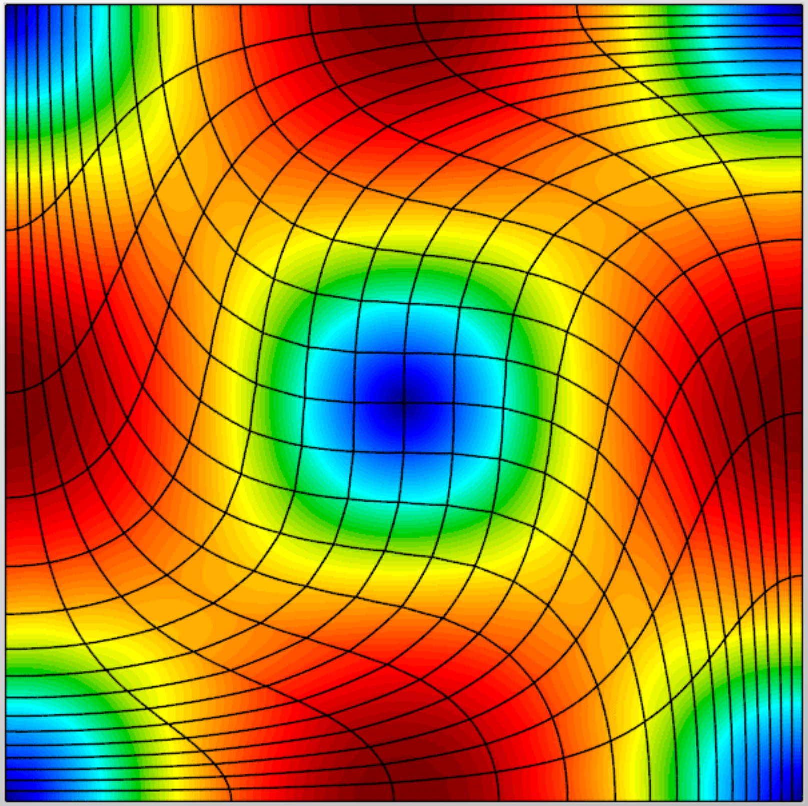


We get 2nd **order convergence for all fields** under mesh refinement (we lose one order in the velocity compared to FEM projection). We get 5th **order remap error** for mass, momentum and total energy.

2D Taylor-Green vortex remap in BLAST



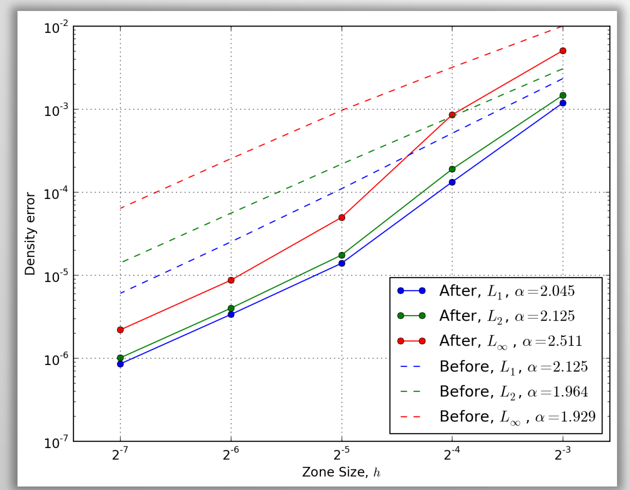
energy, t=0.5

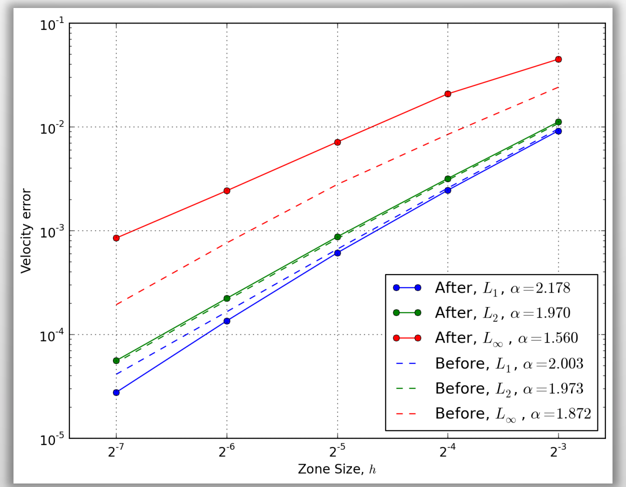


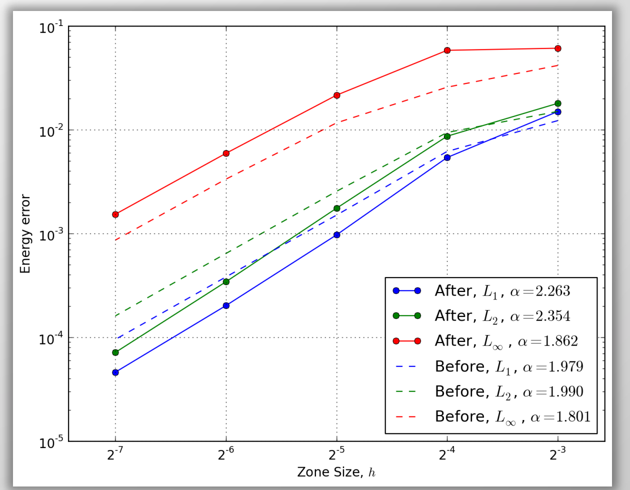
speed, t=0.5

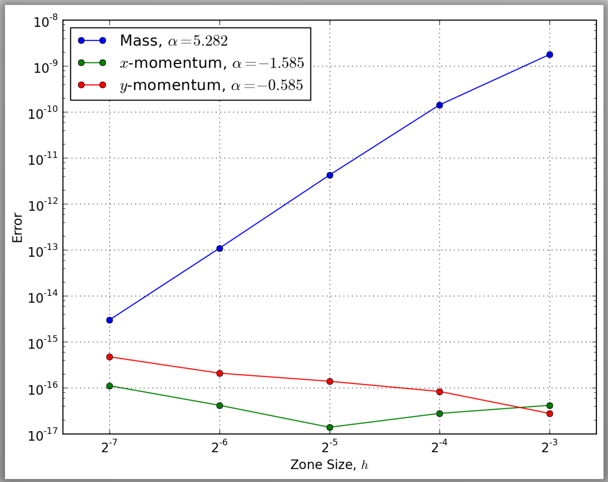
- Q_2-Q_1 method, full mesh relaxation (100 iterations), 30 RK4 steps, no artificial viscosity.
- Simultaneous remap of BLAST-computed Lagrangian high-order mesh and fields.

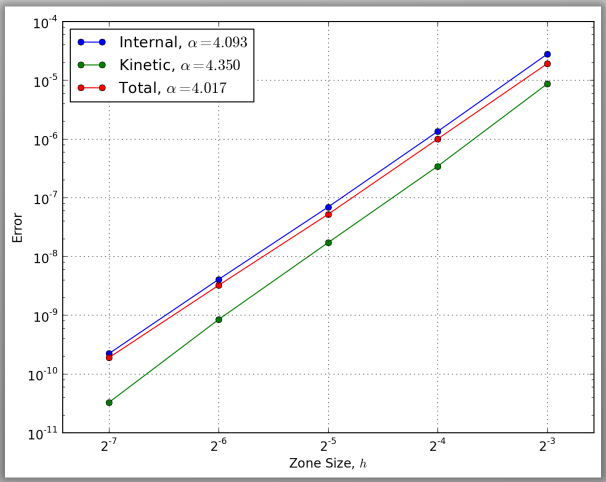
Convergence and errors for the 2D Taylor-Green vortex remap in BLAST with Q_2-Q_1 spaces





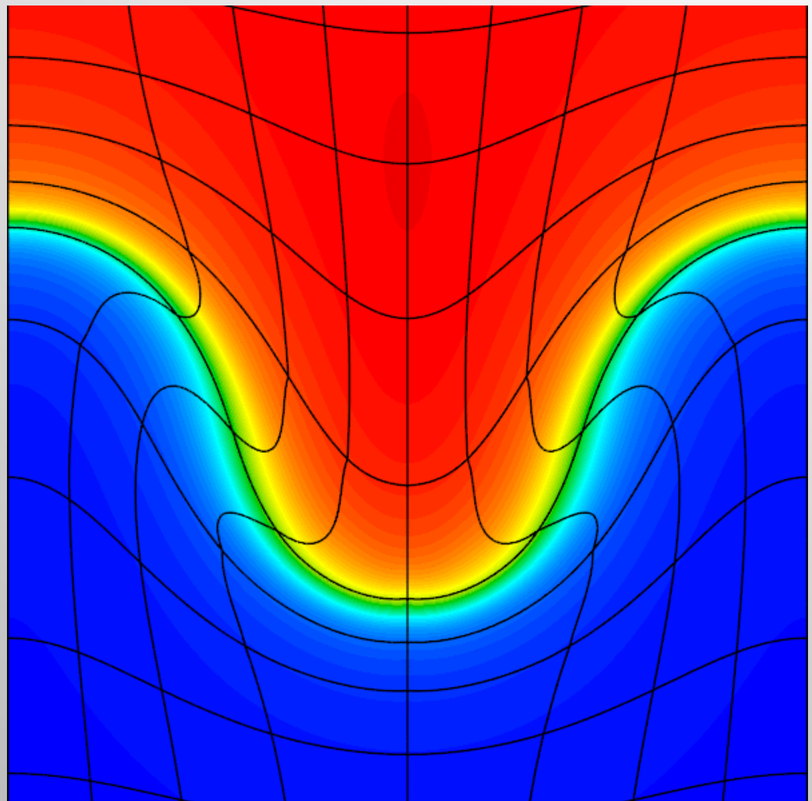




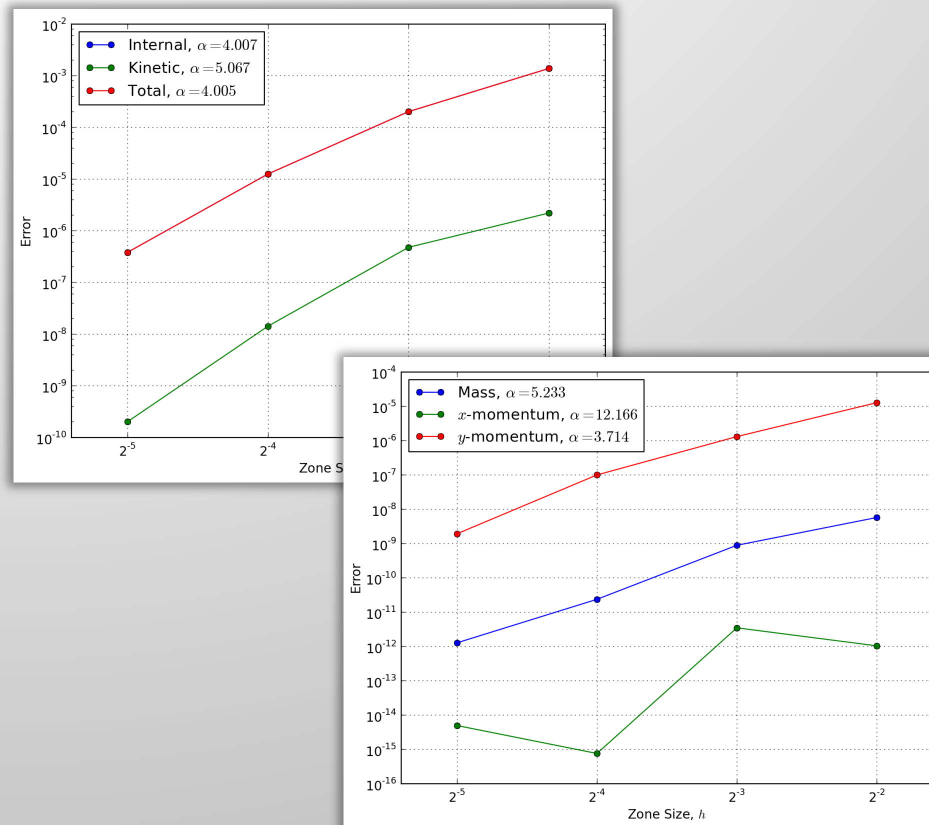


We get 2^{nd} **order convergence for all fields** under mesh refinement, confirming that *the ALE remap matches the accuracy of the Lagrangian method*.
We get **exact momentum**, and **$5^{th}/4^{th}$ order remap err**or for mass and energies.

2D Single-material Rayleigh-Taylor instability remap in BLAST

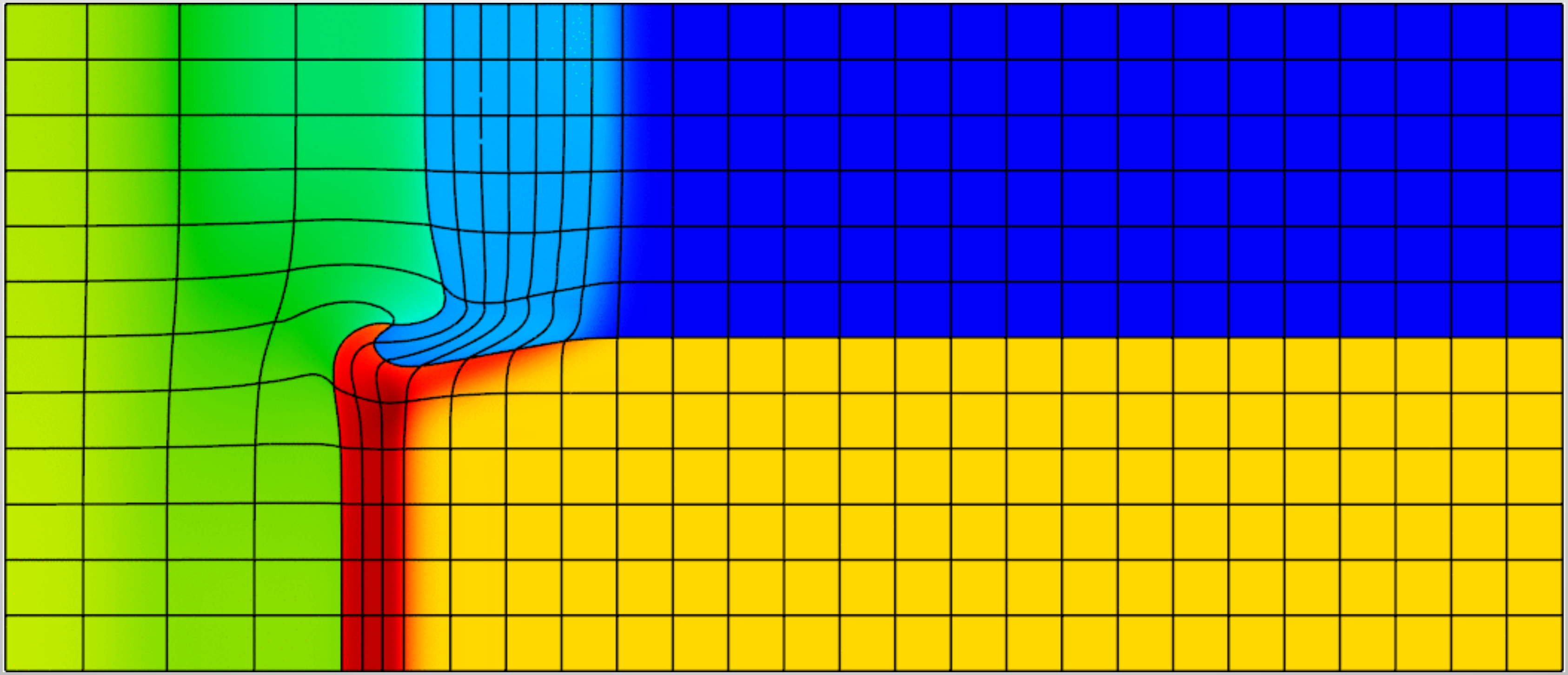


density, t=3



- Q_4-Q_3 method, full mesh relaxation (200 iterations), 50 RK4 steps, no artificial viscosity.
- High-order fields enable accurate representation of sharp transitions inside the zones.
- We get higher-order remap error for mass, momentum and total energy.

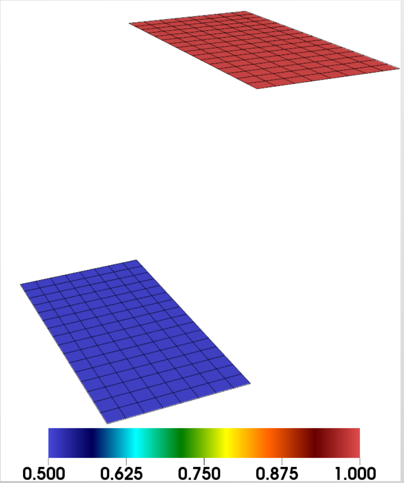
2D Shock triple-point interaction in BLAST

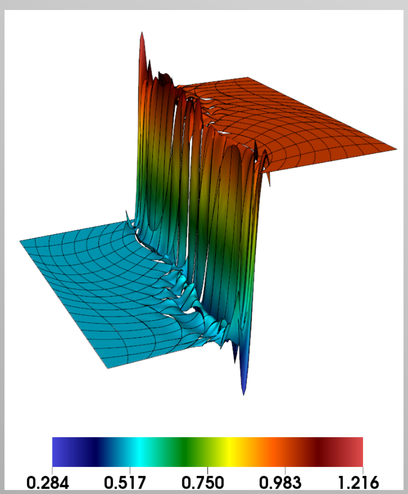


density, t=1

- Q_4-Q_3 method, full mesh relaxation (200 iterations), 50 RK4 steps.
- Preliminary multi-material results. Lack of monotonicity leads to undershoots in density.
- The remap seems to handle reasonably well the presence of shock and material interfaces.

To ensure monotonicity for discontinuous fields, we are exploring ideas from the FCT community





Q_2 remap of a step function

- Monotonicity condition:

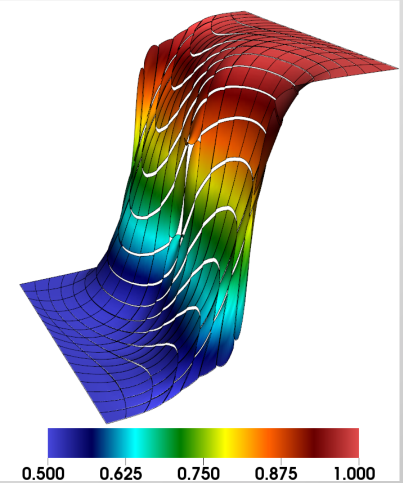
$$\boxed{\frac{\partial \rho_i}{\partial \tau} = \sum_{j \neq i} \mathbf{K}_{ij} \left(\rho_j - \rho_i\right)}$$

with $\mathbf{K}_{ij} \geq 0 \ \ \forall j \neq i$

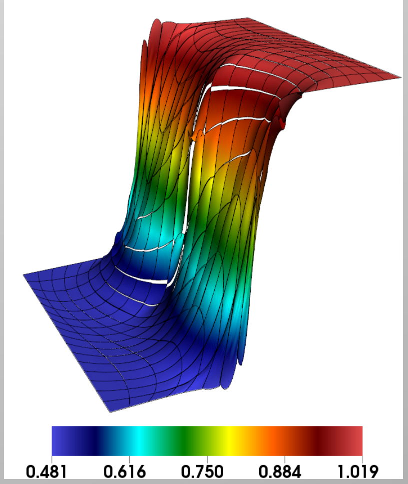
- In the lowest order case, this holds for $\mathbf{K} = -\mathbf{M}^{-1}(\mathbf{A}^{\mathrm{T}} + 2\mathbf{S})$.
- In the high-order case, it can be ensured by "discrete upwinding" but that is too diffusive.
- Algebraic flux-corrected transport (Kuzmin & Turek, 2005):

$$\frac{\partial \rho_i}{\partial \tau} = \sum_{j \neq i} \left(\mathbf{K}_{ij} + (1 - \phi(r_{ij}))\mathbf{D}_{ij}\right) \left(\rho_j - \rho_i\right)$$

- We have adapted this to high-order discontinuous spaces, but more work is needed (mass lumping, FEM basis,…)



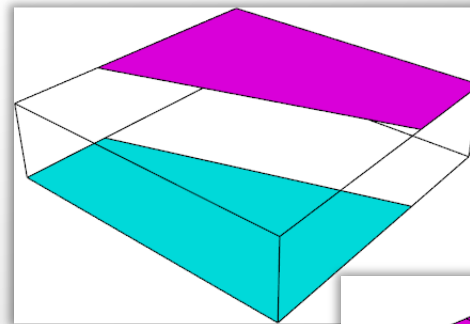
discrete upwinding



algebraic FCT

Current and future work

- Preliminary results with high-order ALE remesh+remap are promising.
- More work is needed to:
  - ensure monotonicity of the remap of high-order discontinuous fields
    (we plan to consider both algebraic and functional approaches)
  - automate the integration in pseudo-time
  - handle zones with mixed materials
    (we plan to investigate high-order material indicator functions)
- Some other recent work in BLAST:
  - High-order FEM hyperviscosity as a limiter and new art. viscosity option (with A.Long, TAMU)
  - GPU/multi-core acceleration on heterogeneous computer architectures (with T.Dong, UTK)



Simple material indicator function and its monotone projection with a Bernstein basis.