Lawrence Livermore National Laboratory

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Scalable High-Order Finite Elements for Compressible Hydrodynamics

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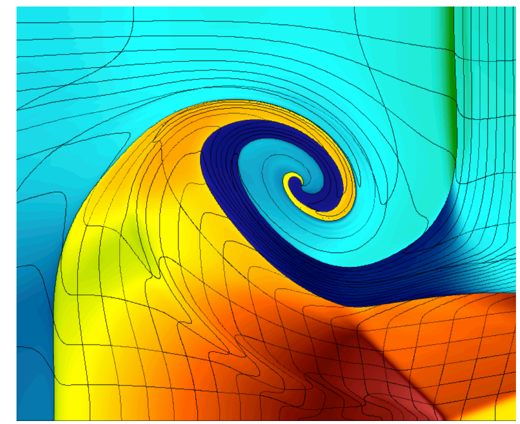
High-order finite elements are a good foundation for next-generation scalable multi-physics simulations

- Large-scale parallel multi-physics simulations
  - radiation diffusion
  - electromagnetic diffusion
  - compressible hydrodynamics
- Finite elements naturally connect different physics

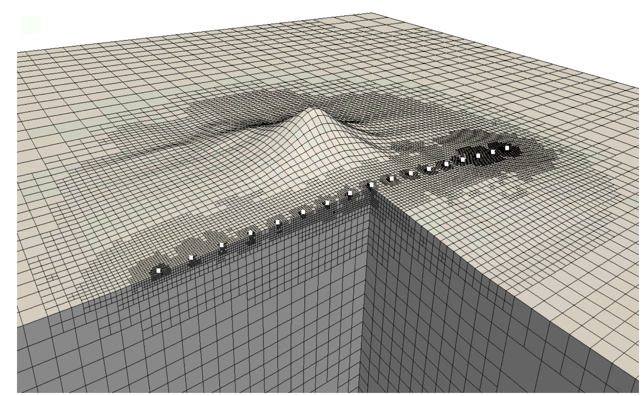
$$H(grad) \xrightarrow{\nabla} H(curl) \xrightarrow{\nabla\times} H(div) \xrightarrow{\nabla\cdot} L_2$$

$H(grad)$	$H(curl)$	$H(div)$	L_2
"nodes"	"edges"	"faces"	"zones"
High-order kinematics	High-order MHD	High-order rad. diff.	High-order thermodynamics



8^{th} order Lagrangian hydro simulation of a shock triple-point interaction

- High-order finite elements on high-order meshes
  - increased accuracy for smooth problems
  - sub-element modeling for problems with shocks
  - bridge unstructured/structured, sparse/dense
  - FLOPs/bytes increase with the order
- Need new (interesting!) R&D for full benefits
  - meshing, discretizations, solvers, AMR, UQ, visualization, …



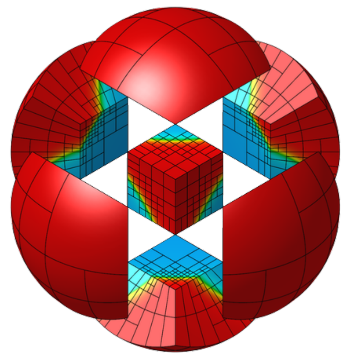
High-order H(curl) AMR in geophysics modeling of subsurface electric conductivity

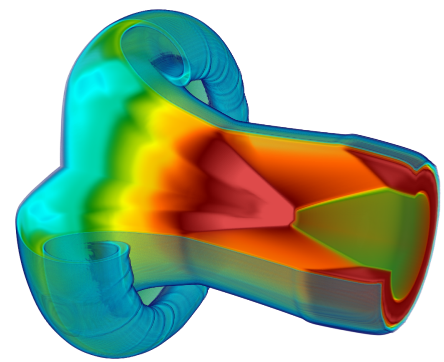
Our scalable high-order finite element simulation pipeline

hypre: *Scalable linear solvers library*

MFEM: *Modular finite element methods library*

BLAST: *High-order ALE shock hydrodynamics research code*





www.llnl.gov/casc/hypre

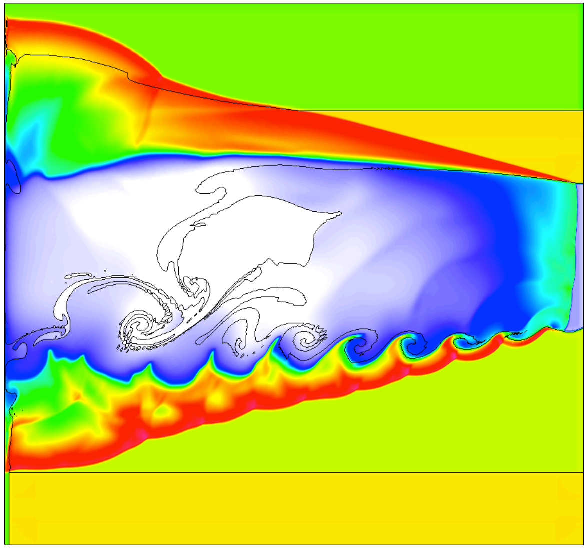
mfem.org

www.llnl.gov/casc/blast

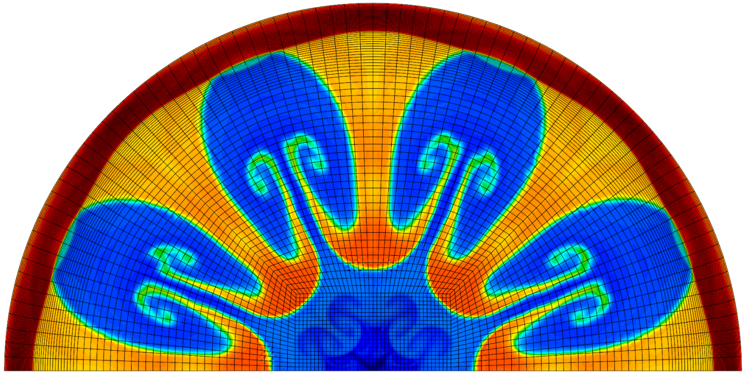
- FE research and fast application prototyping – MFEM
- High-order hydrodynamics and multi-physics – BLAST
- Scalable solvers for radiation, electromagnetic diffusion – *hypre*

Compressible shock hydrodynamics

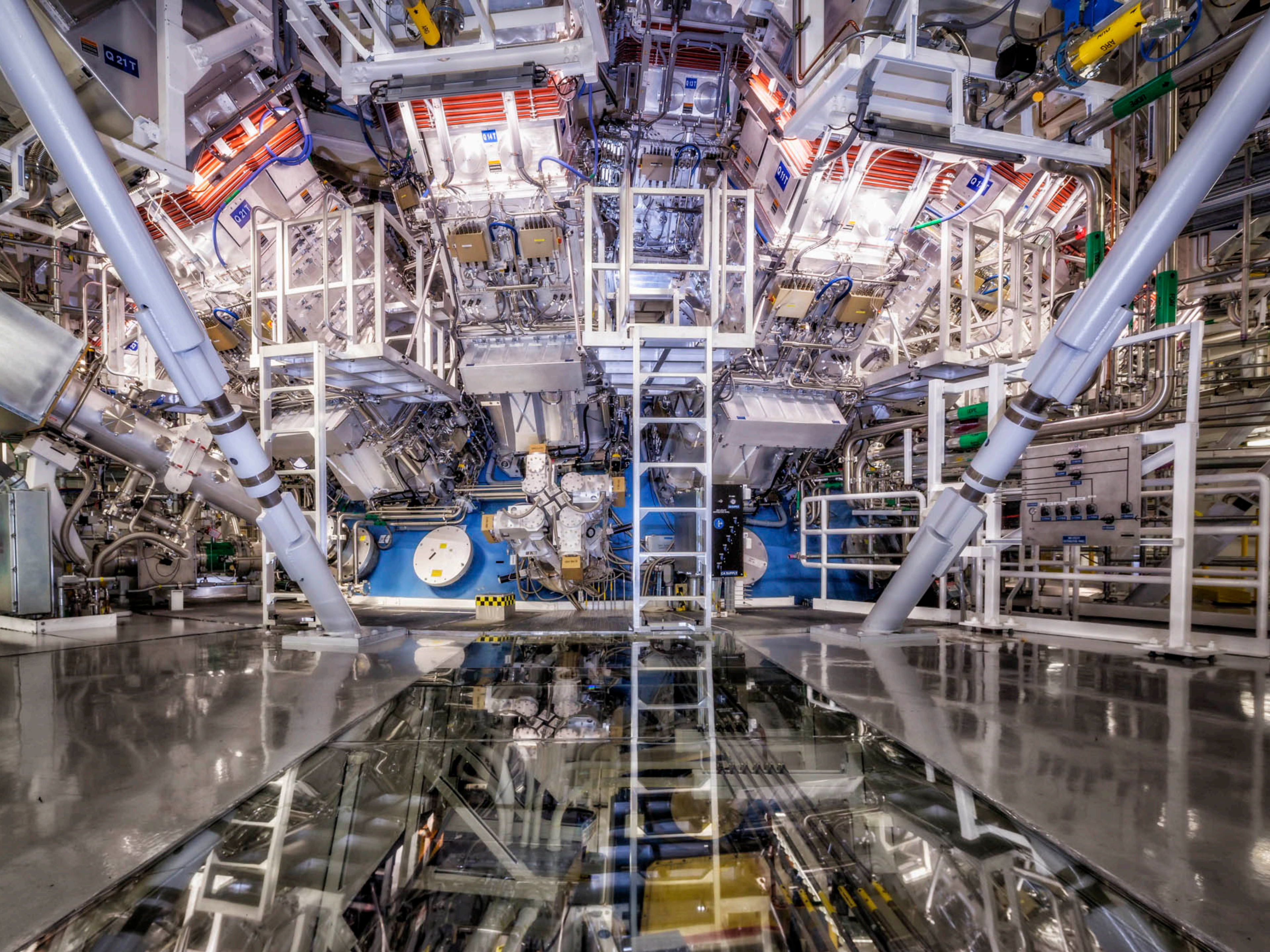
- Compressible Hydrodynamics describes flows where the density changes in response to pressure.
- This is the case in gases, or liquids with large energies and/or pressure changes.
- Many applications at LLNL/DOE, e.g. implosion in the National Ignition Facility.
- Mathematical challenges:
  - shock waves
  - handling of discontinuous solutions
  - moving meshes
  - multi-material flow
  - coupling with other physics



Laser-driven high energy-density plasma computation



Inertial Confinement Fusion


Q 21T

ALE Discretizations for Large-Scale Hydrodynamic Simulations

The Arbitrary Lagrangian-Eulerian (ALE) framework 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: $\frac{\mathrm{d}\rho}{\mathrm{d}t} + \vec{c}\cdot\nabla\rho = -\rho\nabla\cdot\vec{v}$

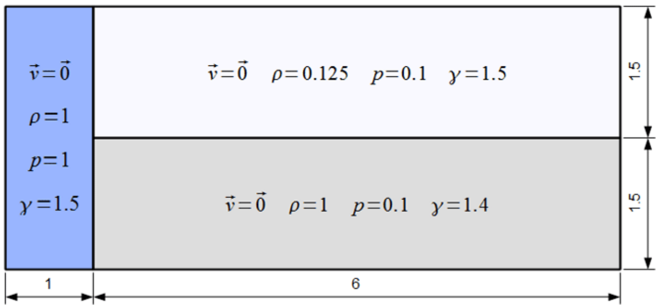
Energy Conservation: $\rho\left(\frac{\mathrm{d}e}{\mathrm{d}t} + \vec{c}\cdot\nabla e\right) = \sigma : \nabla\vec{v}$

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

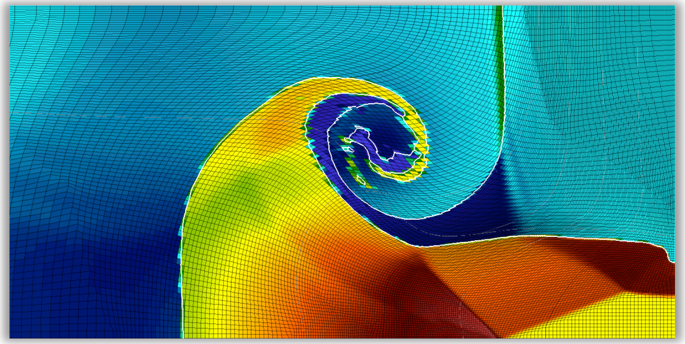
Equation of Motion: $\frac{\mathrm{d}\vec{x}}{\mathrm{d}t} + \vec{c} = \vec{v}$

Typical ALE approaches for shock hydro consist of:

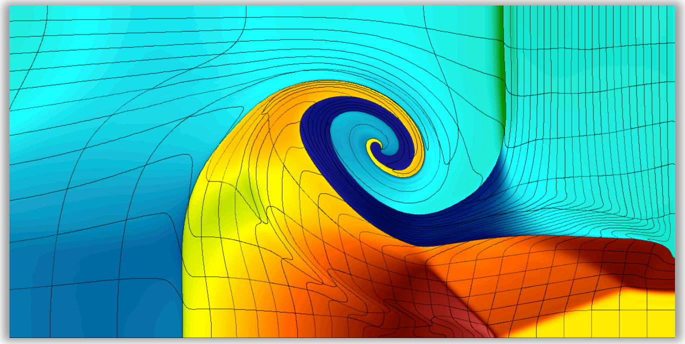
- Lagrangian phase
  - Moving computational mesh
- Advection phase
  - Mesh optimization
  - Conservative field remap
  - Monotonicity
- Multi-material element treatment



Triple-point shock interaction problem



Traditional ALE simulation

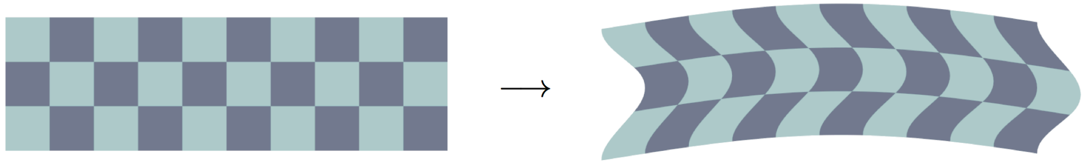


High-order Lagrangian simulation

The BLAST code discretizes the ALE fields and geometry with high-order finite elements

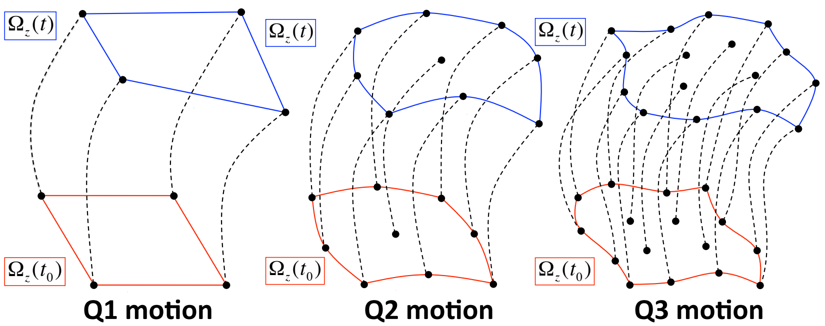
BLAST – novel simulation code combining:

- *High-order finite elements* +
- *High-order meshes* +
- *ALE hydrodynamics*



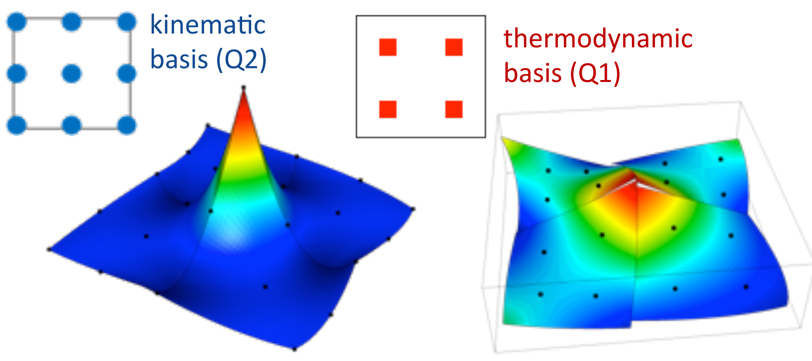
Lagrange Phase

- Solve hydro PDEs on moving curvilinear mesh
- Continuous HO kinematics
- Discontinuous HO materials and thermodynamics
- HO extension of classical SGH



Remap Phase

- HO mesh optimization
- Field remap by solving advection in pseudo-time
- Ensure conservation and HO monotonicity



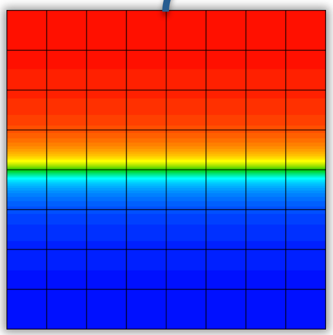
We models shock hydrodynamics using high-order FEM in both Lagrangian and Remap phases

<u>Lagrangian phase</u>

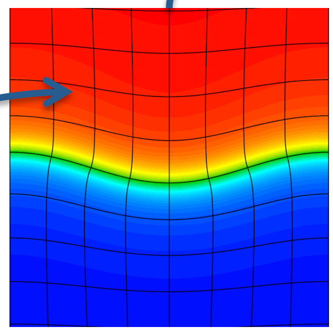
- mesh motion determined by physical velocity
- time t evolution

<u>Remap phase</u>

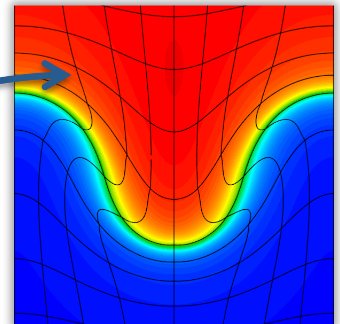
- artificial mesh motion, defining the mesh velocity
- "pseudo-time" τ evolution



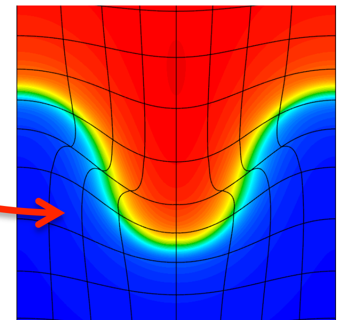
$t = 0$



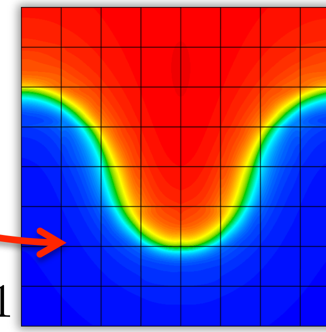
$t = 1.5$



$t = 3.0 \quad \tau = 0$

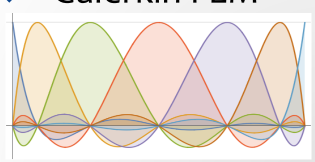


$\tau = 0.5$



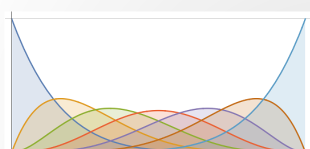
$\tau = 1$

- Galerkin FEM



Gauss-Lobatto basis

- DG FEM



Bernstein basis

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

Momentum Conservation: $\rho \dfrac{\mathrm{d}\vec{v}}{\mathrm{d}t} = \nabla \cdot \sigma$

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

Energy Conservation: $\rho \dfrac{\mathrm{d}e}{\mathrm{d}t} = \sigma : \nabla \vec{v}$

Equation of Motion: $\dfrac{\mathrm{d}\vec{x}}{\mathrm{d}t} = \vec{v}$

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

Momentum Conservation: $\dfrac{\mathrm{d}(\rho\vec{v})}{\mathrm{d}\tau} = \vec{v}_m \cdot \nabla(\rho\vec{v})$

Mass Conservation: $\dfrac{\mathrm{d}\rho}{\mathrm{d}\tau} = \vec{v}_m \cdot \nabla \rho$

Energy Conservation: $\dfrac{\mathrm{d}(\rho e)}{\mathrm{d}\tau} = \vec{v}_m \cdot \nabla(\rho e)$

Mesh velocity: $\vec{v}_m = \dfrac{\mathrm{d}\vec{x}}{\mathrm{d}\tau}$

We represent different materials as high-order material indicator functions

- Mixed cells appear after remap or due to shaping
  - ✓ *different material properties, but one velocity*

- We track materials with material indicator functions:

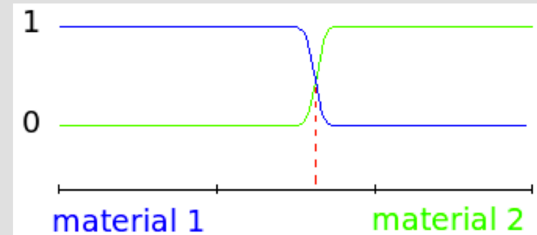
$$\eta_k \approx \frac{V_k}{V}, \quad \sum_k \eta_k = 1, \quad 0 \leq \eta_k(x,t) \leq 1.$$

  - ✓ Finite element functions or sub-cell point values
  - ✓ High-order generalization of "volume fractions"

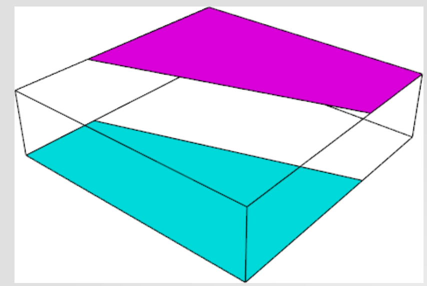
- Volume change is controlled by the volumetric strain

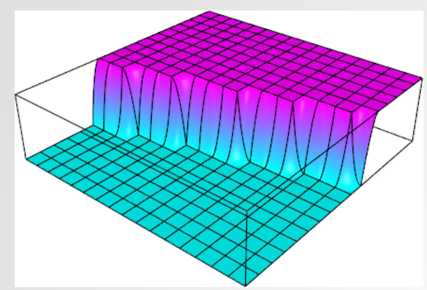
$$\beta_k \approx \frac{dV_k}{dV}, \quad \sum_k \beta_k = 1$$

  - ✓ *Lagrangian indicators:* $\beta_k = \eta_k$
  - ✓ *Closure models: sub-zonal strain evolution*



Indicators for a two-material problem in 1D





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

Lagrange phase solves a system of conservation laws in physical time using Galerkin finite elements

Continuous Lagrange

Material indicators
$$\frac{d\eta_k}{dt} = (\beta_k - \eta_k)\nabla \cdot v$$

Material mass
$$\int_V \eta_k \rho_k = \int_{V^0} \eta_k^0 \rho_k^0$$

Material energy
$$\eta_k \rho_k \frac{de_k}{dt} = \eta_k \sigma_k : \nabla v$$

Momentum
$$\rho \frac{dv}{dt} = \nabla \cdot \sigma$$

Position
$$\frac{dx}{dt} = v$$

Semi-discrete Lagrange

HO closure model
$$\mathbf{M} \frac{\mathrm{d}\boldsymbol{\eta}_k}{\mathrm{d}t} = \mathbf{b}_k$$

Strong mass conservation
$$\eta_k \rho_k |\mathbf{J}| = \eta_k^0 \rho_k^0 |\mathbf{J}^0|$$

Dense solve
$$\mathbf{M_e} \frac{\mathrm{d}\mathbf{e}_k}{\mathrm{d}t} = \mathbf{F}_k^T \cdot \mathbf{v}$$

Sparse solve
$$\mathbf{M_v} \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\mathbf{F} \cdot \mathbf{1}$$

Mesh update
$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}$$

Total density
$$\rho \equiv \sum_k \eta_k \rho_k$$

Total internal energy
$$\rho e \equiv \sum_k \eta_k \rho_k e_k$$

Total stress
$$\sigma \equiv \sum_k \eta_k \sigma_k$$

Material mass
$$M_k = \int_\Omega \eta_k \rho_k$$

Material internal energy
$$IE_k = \int_\Omega \eta_k \rho_k e_k$$

Material volume
$$V_k = \int_\Omega \eta_k$$

Zonal thermodynamic mass matrix
$$(\mathbf{M}_{\mathbf{e},k})_{ij} = \int_\Omega \eta_k \rho_k \phi_i \phi_j$$

Generalized corner forces
$$\mathbf{F} = \sum_k \mathbf{F}_k$$

Global kinematic mass matrix
$$(\mathbf{M_v})_{ij} = \int_\Omega \rho w_j w_i$$

Material corner forces
$$(\mathbf{F}_k)_{ij} = \int_\Omega (\eta_k \sigma_k : \nabla w_i)\phi_j$$

* V. Dobrev, Tz. Kolev, R. Rieben, ***"High-order curvilinear finite elements for Lagrangian hydrodynamics"***, SISC, 2012

We have developed a high-order "pseudo-time" DG advection algorithm for conservative and accurate remap

Advection-based remap

- Continuous transition in pseudo-time from the old to the new, optimized, mesh
- Preserve (discontinuous) fields in physical space while the mesh is moving

$$\boxed{\frac{\partial \rho}{\partial \tau} = 0 \Leftrightarrow \frac{d\rho}{d\tau} = u \cdot \nabla \rho} \qquad u = \frac{dx}{d\tau}$$

Accuracy & Conservation

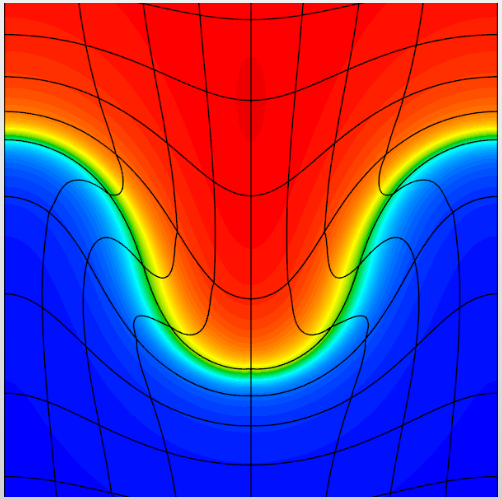
- Discontinuous Galerkin (DG) discretization, upwind flux

$$\frac{\partial}{\partial \tau} \int_\Omega \rho\psi = -\sum_T \int_T \rho u \cdot \nabla \psi + \sum_f \int_f \{\rho u \cdot n\}_* [\![\psi]\!]$$

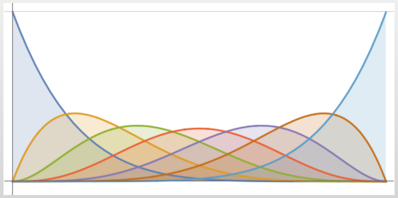
- Remap by ODE integration (swept volumes)
- Order independent, no interface reconstruction

Monotonicity

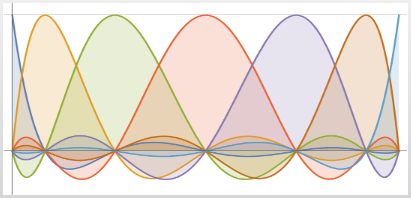
- Preserve bounds, no spurious oscillations
- Enforced at degrees of freedom
- Different approaches: LSD, FCT, and OBR



3rd order DG remap on a 4th order mesh deforming in pseudo-time



Bernstein HO basis: $\eta_k\,,\eta_k\rho_k\,,\eta_k\rho_k e_k$



Gauss-Lobatto HO basis v_x, v_y, v_z

Remap phase solves a system of advection equations in pseudo time using Discontinuous Galerkin finite elements

	Continuous Remap	Semi-discrete Remap	
Material indicators	$\frac{d\eta_k}{d\tau} = u \cdot \nabla \eta_k$	$\mathbf{M}\frac{\mathrm{d}\boldsymbol{\eta}_k}{\mathrm{d}\tau} = \mathbf{K}\boldsymbol{\eta}_k$	
Material mass	$\frac{d(\eta_k \rho_k)}{d\tau} = u \cdot \nabla(\eta_k \rho_k)$	$\mathbf{M}\frac{\mathrm{d}(\boldsymbol{\eta\rho})_k}{\mathrm{d}\tau} = \mathbf{K}(\boldsymbol{\eta\rho})_k$	*Assembly & dense solve*
Material energy	$\frac{d(\eta_k \rho_k e_k)}{d\tau} = u \cdot \nabla(\eta_k \rho_k e_k)$	$\mathbf{M}\frac{\mathrm{d}(\boldsymbol{\eta\rho e})_k}{\mathrm{d}\tau} = \mathbf{K}(\boldsymbol{\eta\rho e})_k$	
Momentum	$\frac{d(\rho v)}{d\tau} = u \cdot \nabla(\rho v)$	$\mathbf{M_v}\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}\tau} = \mathbf{K_v}\mathbf{v}$	*Assembly & sparse solve*
Remesh velocity	$\frac{dx}{d\tau} = u$	$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\tau} = \mathbf{u}$	*Remesh update*

Zonal thermodynamic mass matrix

$$\mathbf{M}_{ij} = \int_\Omega \phi_j \phi_i$$

Global kinematic mass matrix

$$(\mathbf{M_v})_{ij} = \int_\Omega \rho w_j w_i$$

Thermodynamic advection matrix

$$\mathbf{K}_{ij} = \sum_z \int_z \mathbf{u} \cdot \nabla \phi_j \phi_i - \sum_f \int_f (\mathbf{u} \cdot \mathbf{n}) [\![\phi_j]\!] (\phi_i)_d$$

Kinematic advection matrix

$$(\mathbf{K_v})_{ij} = \int_\Omega \rho\, \mathbf{u} \cdot \nabla w_j \cdot w_i$$

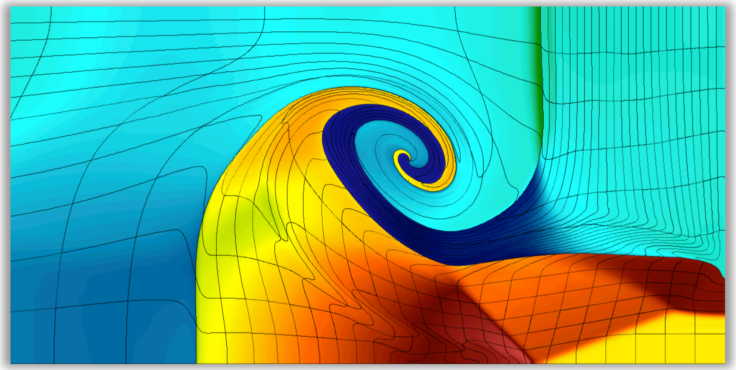
* R. Anderson, V. Dobrev, Tz. Kolev, R. Rieben, ***"Monotonicity in high-order curvilinear finite element arbitrary Lagrangian–Eulerian remap"***, IJNMF, 2015

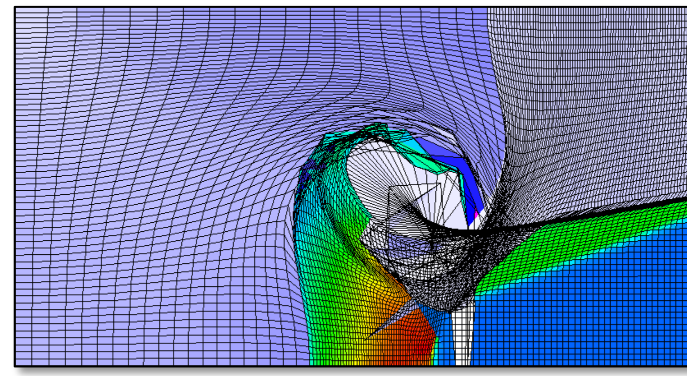
High-order FE on high-order meshes lead to more robust and reliable Lagrangian simulations

High-order

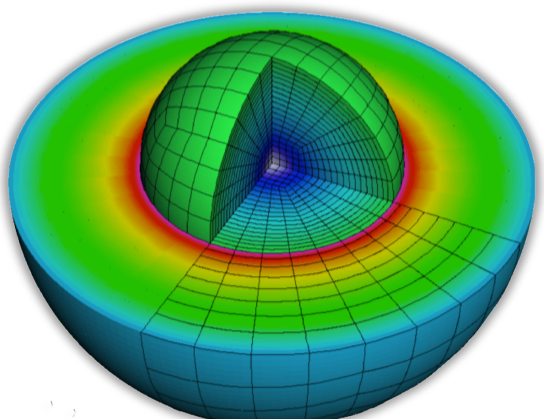
Low-order SGH

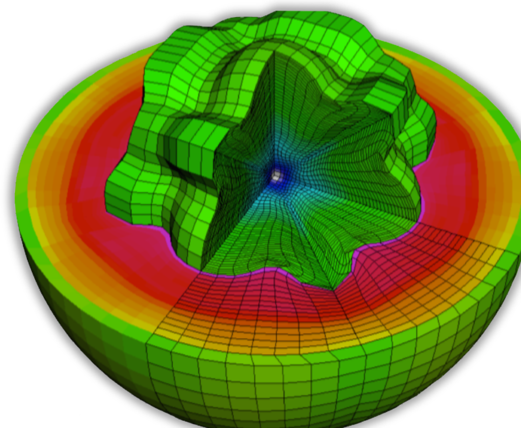
Robustness



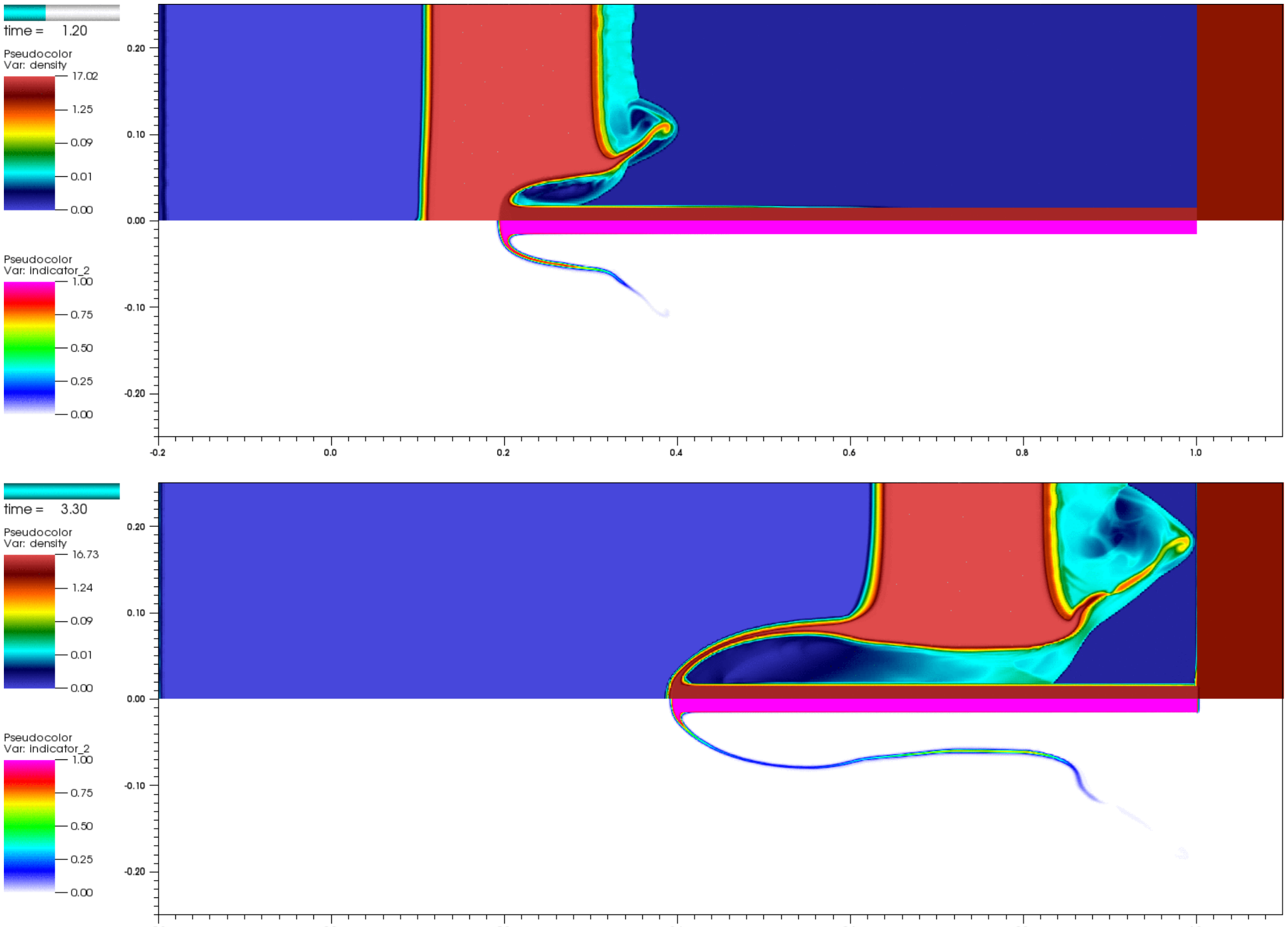


Symmetry preservation

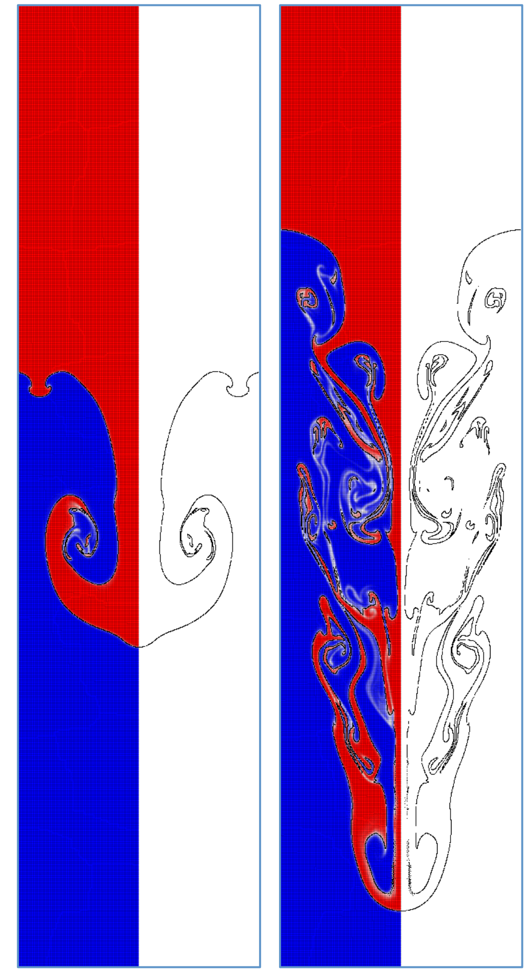




High-order methods perform well on a variety of challenging multi-material ALE problems



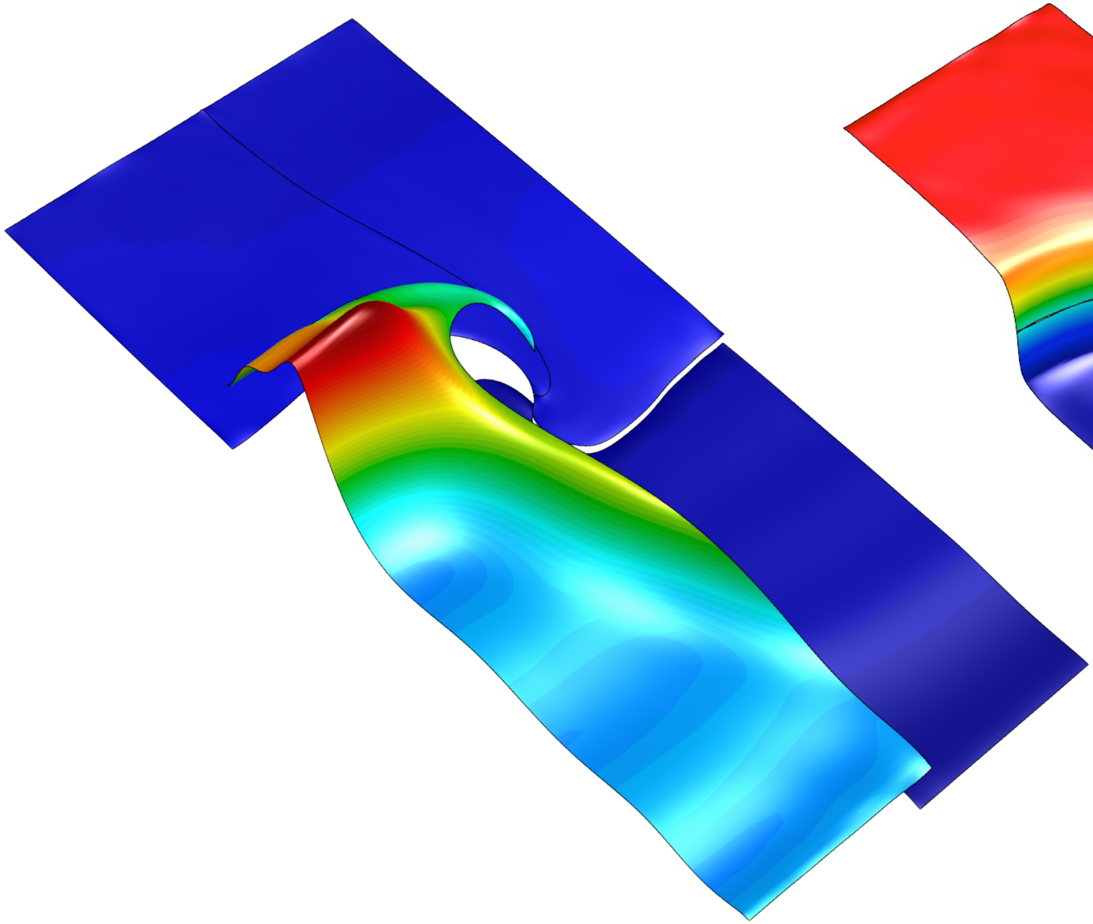
4-material axisymmetric high-velocity plate/rod impact



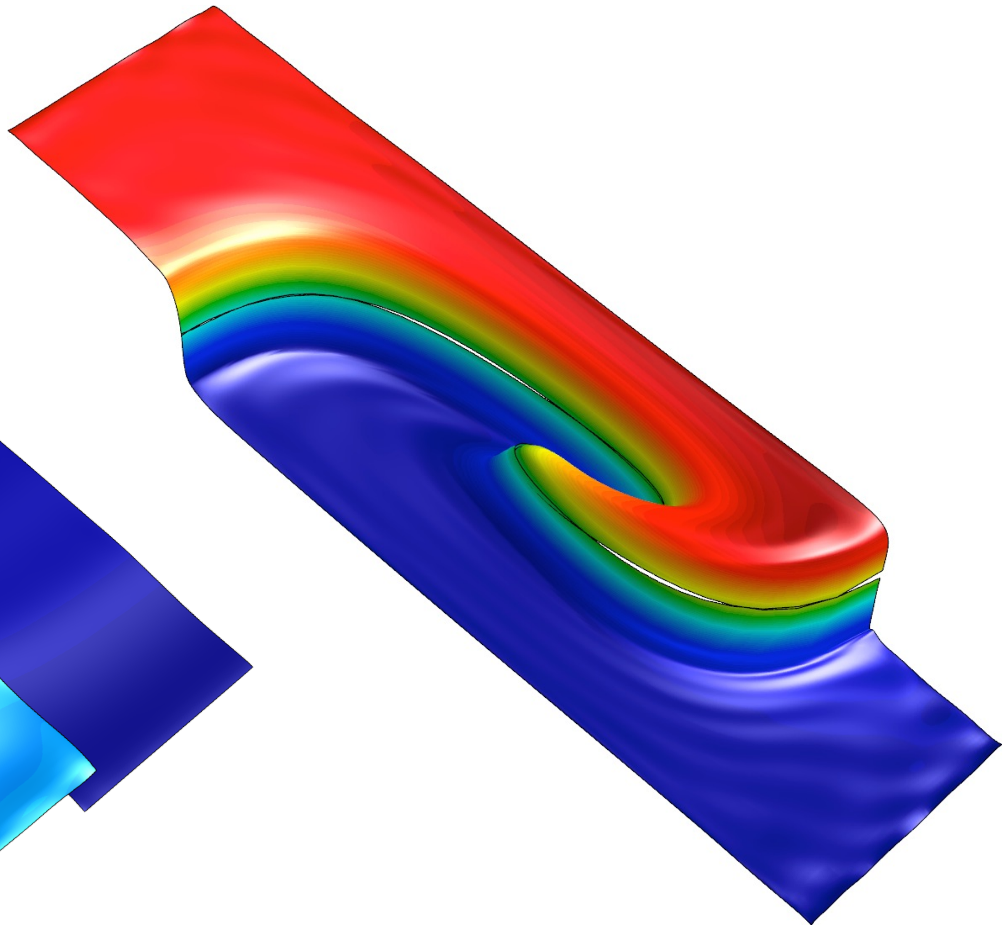
2-material RT instability

Lagrangian simulations on coarse meshes with Q12-Q11 finite elements

Lagrangian simulations on coarse meshes with Q12-Q11 finite elements



Shock triple-point interaction (4 elements)



Smooth RT instability (2 elements)

Semi-discrete Lagrangian phase and its finite element numerical kernels

Lagrangian algorithm in BLAST

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

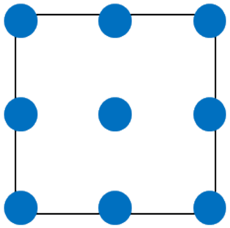
$$\mathbf{M_e}\frac{\mathrm{d}\mathbf{e}}{\mathrm{d}t} = \mathbf{F^T}\cdot\mathbf{v}$$

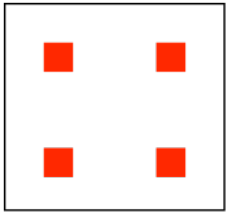
$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}$$

Generalized force matrix

$$\mathbf{F}_{ij} = \int_{\Omega(t)} (\sigma : \nabla \vec{w}_i)\,\phi_j$$

18×4 for Q2-Q1,
32×9 for Q3-Q2,…





Kernel 1: Assembly/evaluation of the zonal corner forces:

$$(\mathbf{F}_z)_{ij} = \int_{\Omega_z(t)} (\sigma : \nabla \vec{w}_i)\,\phi_j = \sum_k \alpha_k \hat{\sigma}(\hat{\vec{q}}_k) : \mathbf{J}_z^{-1}(\hat{\vec{q}}_k)\hat{\nabla}\hat{\vec{w}}_i(\hat{\vec{q}}_k)\,\hat{\phi}_j(\hat{\vec{q}}_k)|\mathbf{J}_z(\hat{\vec{q}}_k)|$$

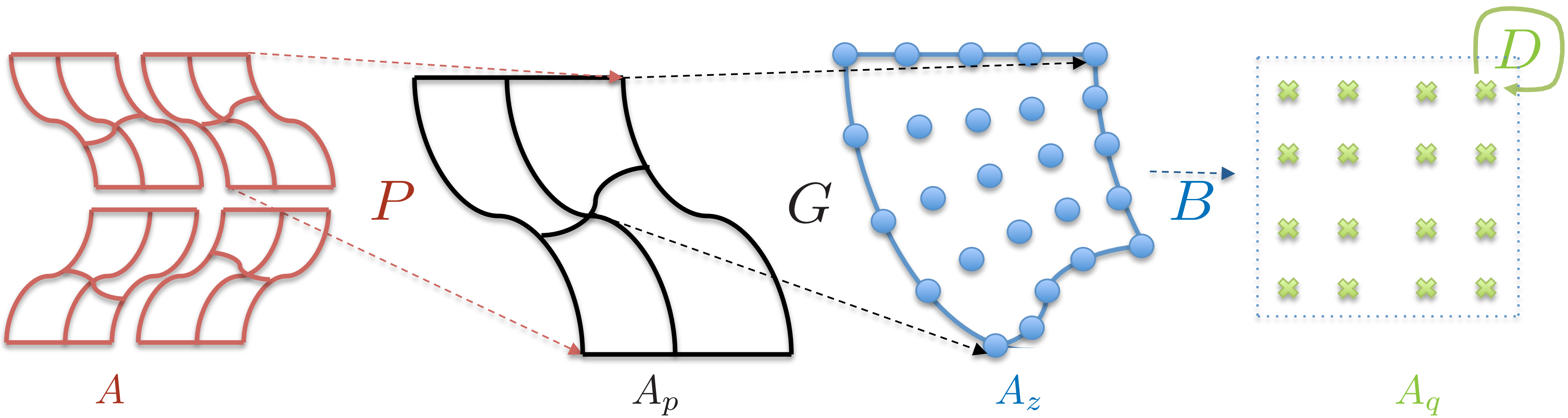
Kernel 2: Inversion of the (global) kinematic mass matrix:

$$(\mathbf{M_v})_{ij} = \int_{\Omega_z} \rho\,\vec{w}_i\cdot\vec{w}_j = \sum_k \alpha_k \hat{\rho}(\hat{\vec{q}}_k)\hat{\vec{w}}_i(\hat{\vec{q}}_k)\cdot\hat{\vec{w}}_j(\hat{\vec{q}}_k)|\mathbf{J}_z(\hat{\vec{q}}_k)|$$

Kernel 1: Partial assembly and evaluation of bilinear forms

$$\boxed{A = P^T G^T B^T D B G P}$$

The finite element assembly/evaluation of general bilinear forms (matrices) can be decomposed into *parallel*, *mesh topology*, *FE basis*, and *geometry/physics* components:

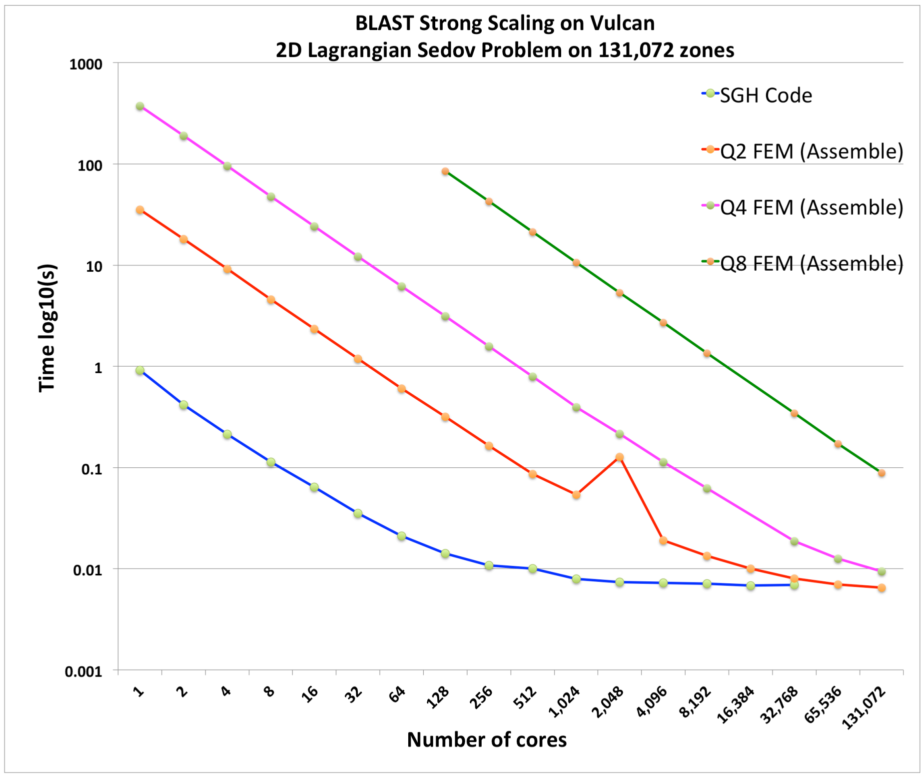


Storage options:

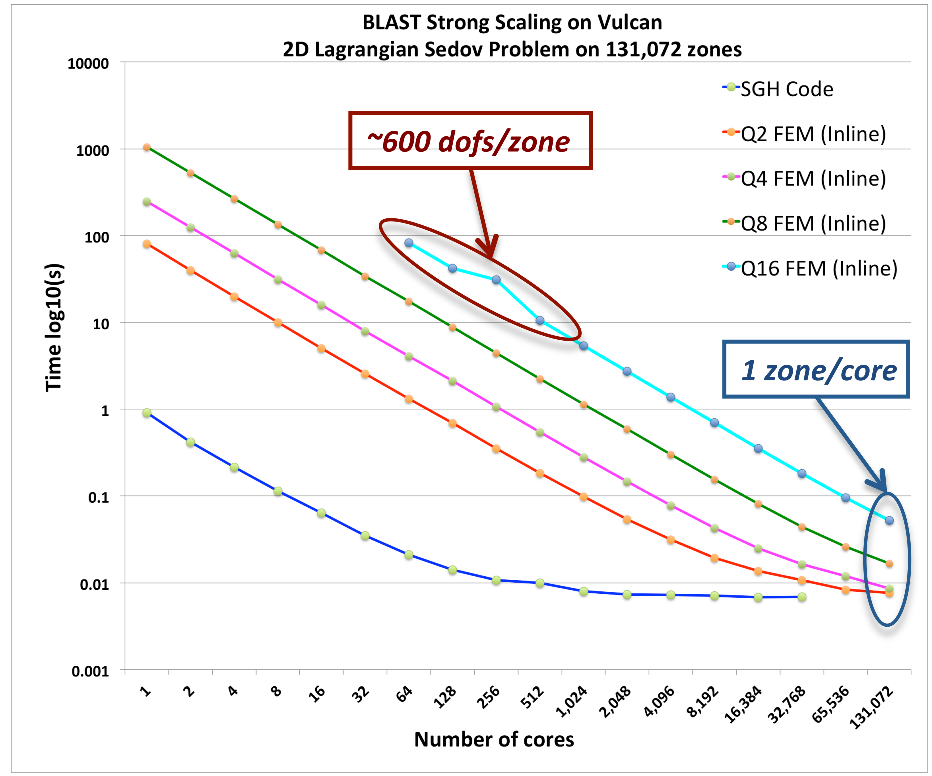
1. A_p, A : standard global matrices (e.g. in CSR/ParCSR format)
2. A_z : local stiffness matrices (e.g. for high-order methods)
3. D : quadrature point data only (independent of basis order)
4. *none* : action-only evaluation (e.g. for explicit methods)

Large-scale strong scalability with partial assembly

Full assembly



Quadrature-point storage only (D_E)



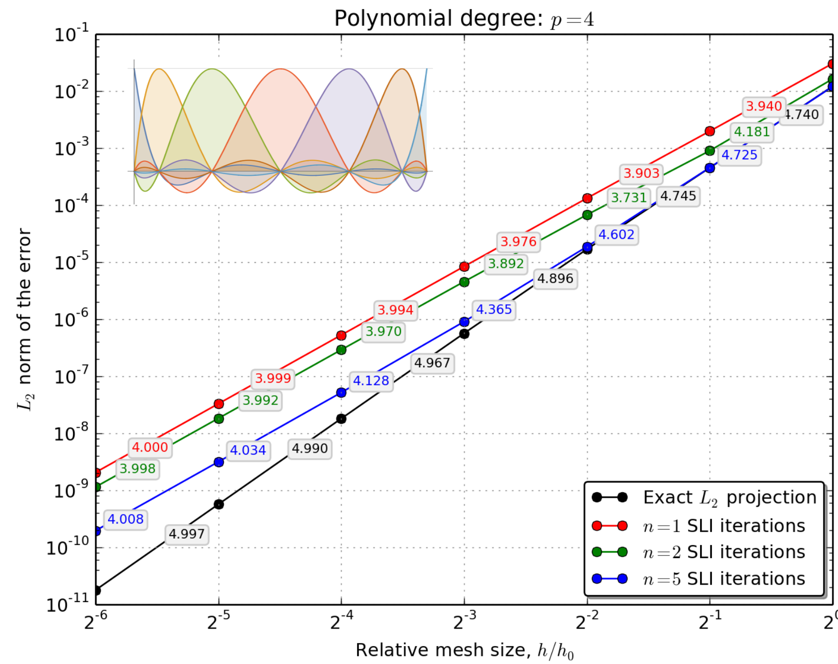
- p-refinement on 512×256 mesh, strong scaling down to 1 elem/core, high-order results in low order run time at 32K cores
- Newer result have much earlier cross-over point
- Quadrature-point storage in mass/corner force matrices, Jacobi preconditioning

Kernel 2: Stationary linear iteration (SLI) approximation

Lumped mass matrix in the Gauss-Lobatto basis is close to the full mass matrix.

A sequence of improving approximations:

- $B_1 = M_L^{-1}$
- $B_2 = 2M_L^{-1} - M_L^{-1} M M_L^{-1}$
- ...
- $I - B_n M = (I - M_L^{-1} M)^n$

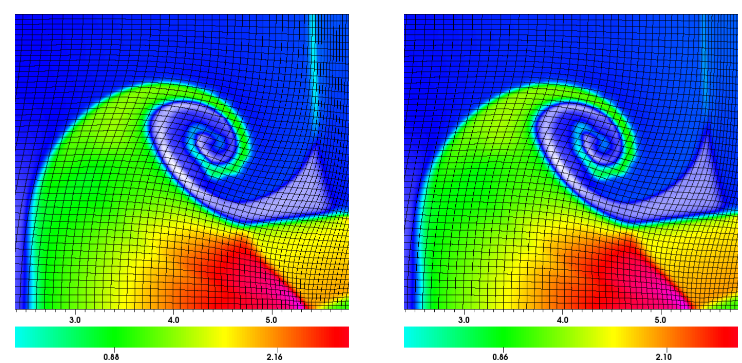


Properties:

- mass conserving: $1^t B_n \rho = 1^t M \rho$
- limited spread of information
- converge to exact inverse: $\lim_{n\to\infty} B_n = M^{-1}$
- equivalent to fixed numbers of stationary linear iterations: $x_n = B_n b$ is the same as

  $$x_0 = 0, \quad x_{k+1} = x_k + M_L^{-1}(b - M x_k)$$

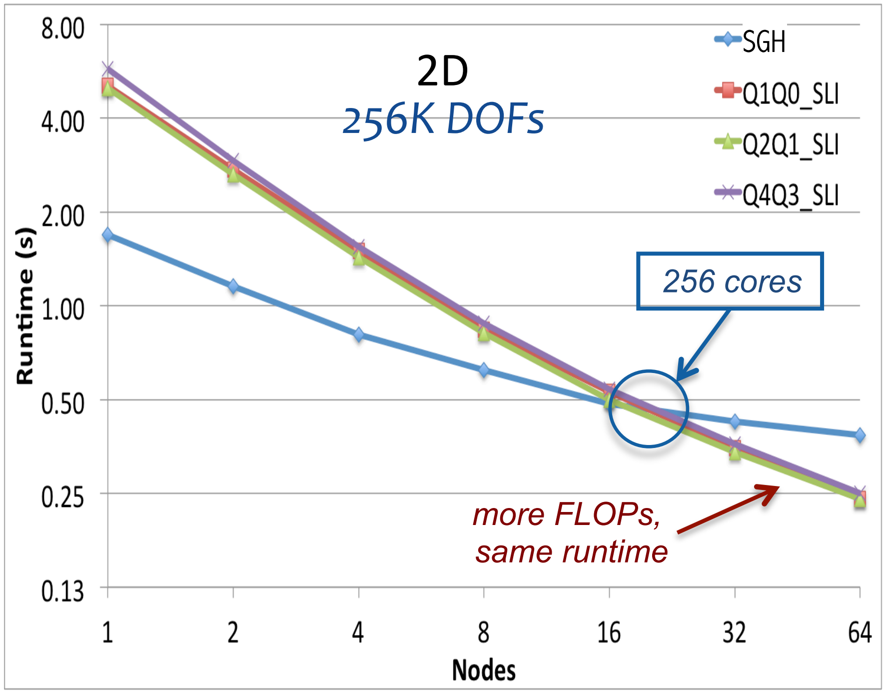
  for $k = 1, \ldots, n$.

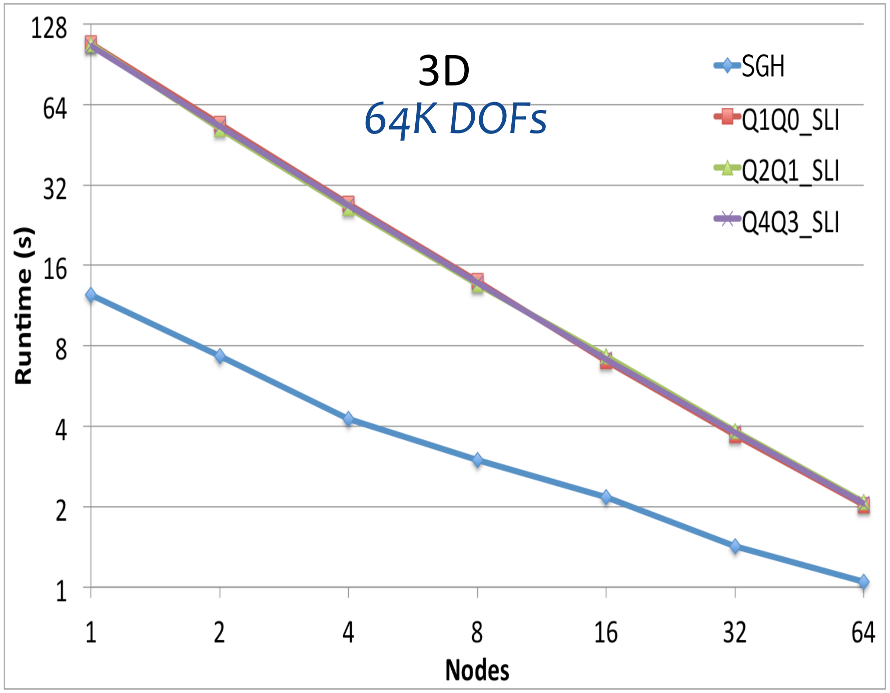


2Drz, 2nd order ALE, PCG (left) vs SLI, n=4 (right)

Recent strong scalability on a BG/Q node with SLI

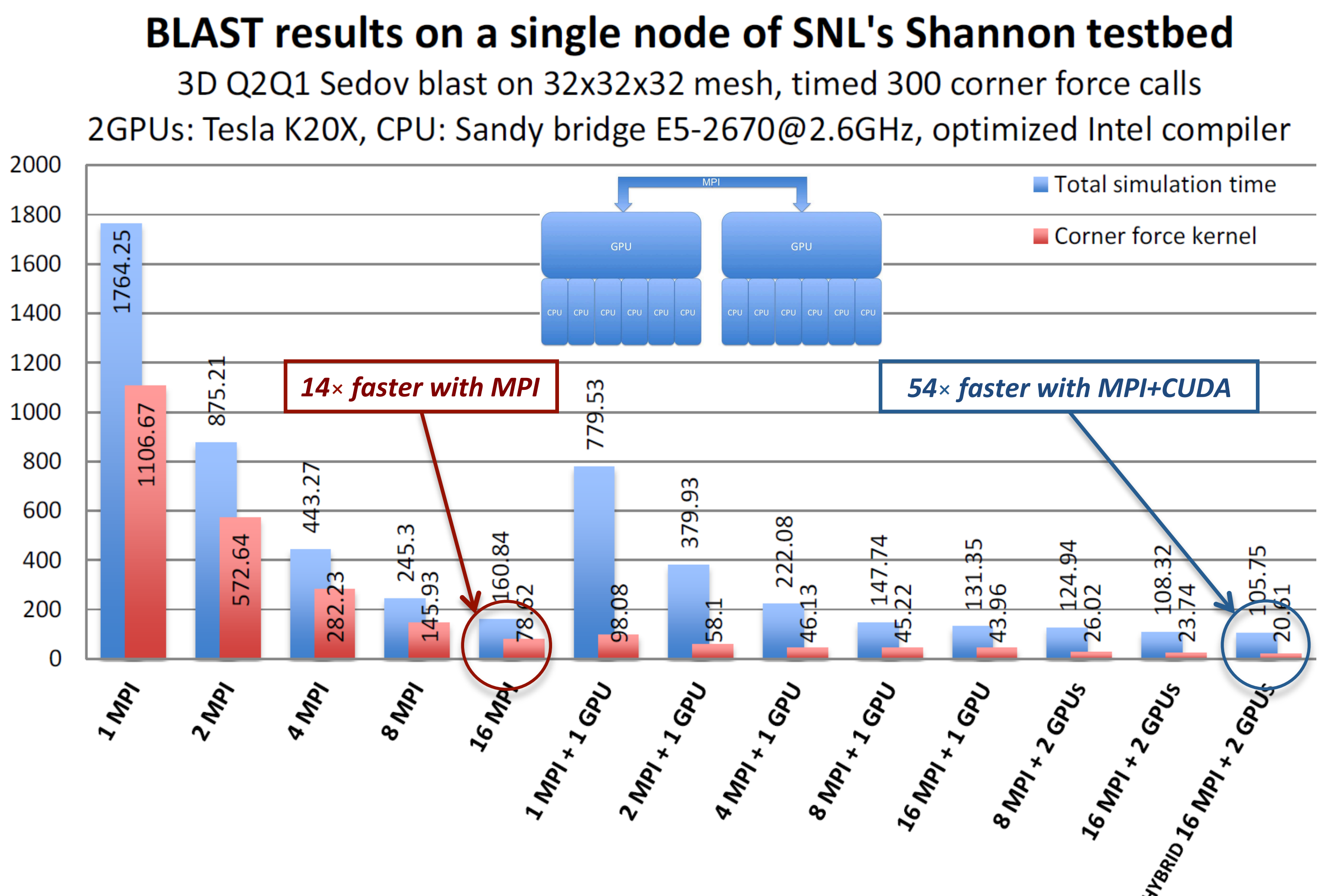
*Lagrangian Sedov problem with **fixed number of DOFs** (different meshes)*





BLAST has good strong scaling properties

High-order finite element kernels are well-suited for GPU acceleration

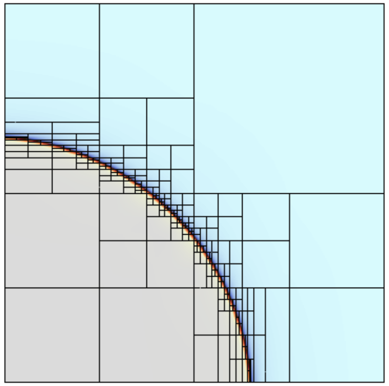


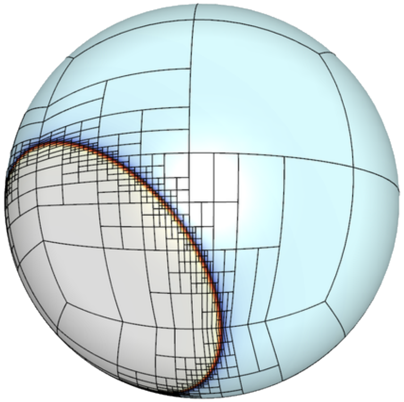
- 6 CUDA kernels, Hyper-Q, CPU-GPU transfer of vectors

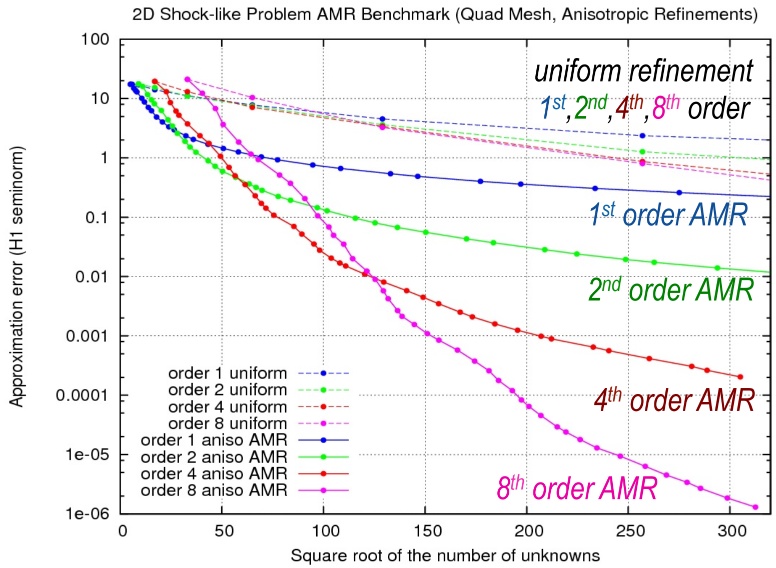
* T. Dong, V. Dobrev, Tz. Kolev, R. Rieben, S. Tomov, J. Dongarra, **"A step towards energy efficient computing: redesigning a hydrodynamic application on CPU-GPU"**, IEEE PDPS, 2014

General adaptive mesh refinement on high-order curved meshes

- Non-conforming refinement for quad/hex meshes is actively developed in MFEM.
  - Implemented by generalizing G, P
  - h-refinement with fixed p
- Powerful and general:
  - any (high-order) finite element space on any (high-order) curved mesh
  - arbitrary order hanging nodes
  - anisotropic refinement
  - serial and parallel (limited)
  - independent of the physics (easy to incorporate in BLAST, etc.)
- **Top**: Adaptation to a shock-like solution.
- **Bottom**: relative AMR error for the 2D problem improves significantly with the order (approaching full h-p refinement)

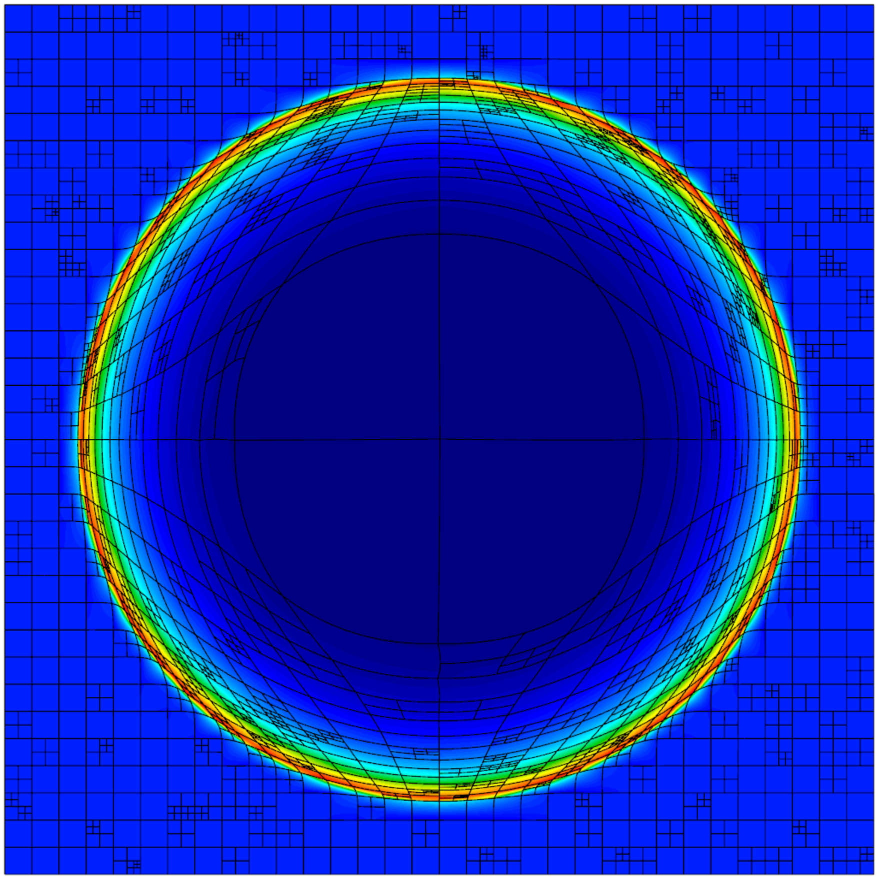




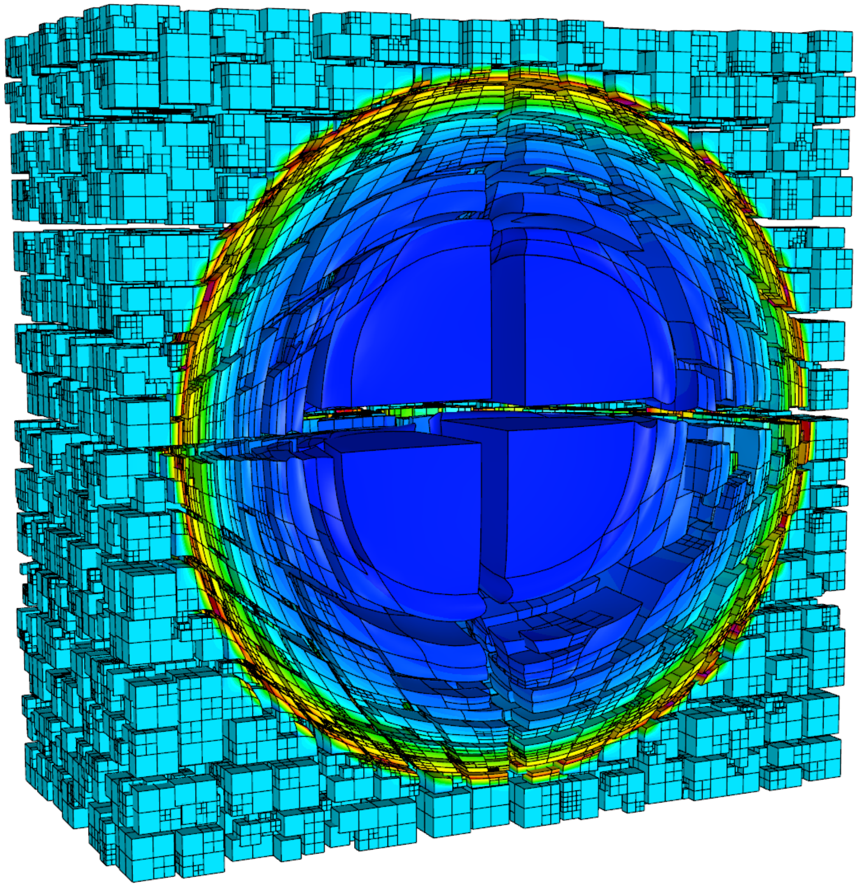


Static parallel NMR, Lagrangian Sedov problem

8 cores, random non-conforming ref.

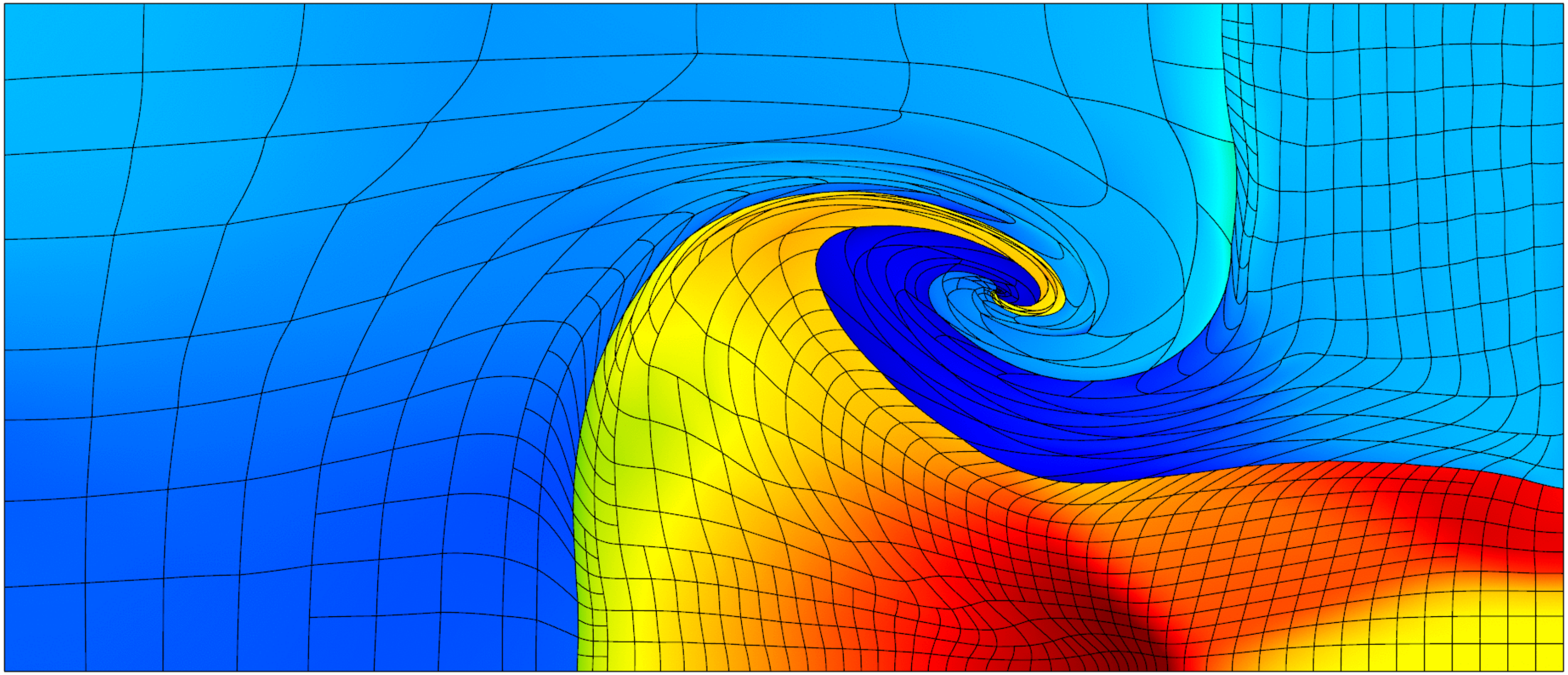


4096 cores, random non-conforming ref.



Shock propagates through non-conforming zones without imprinting

Static parallel AMR, Lagrangian shock triple-point



Anisotropic AMR aiming for "square" elements at t=5.0

Simple anisotropic AMR for high-order H1 and H(curl) problems

- ZZ for (high-order) H1 problems

$$-\nabla \cdot (\rho \nabla u) = f$$

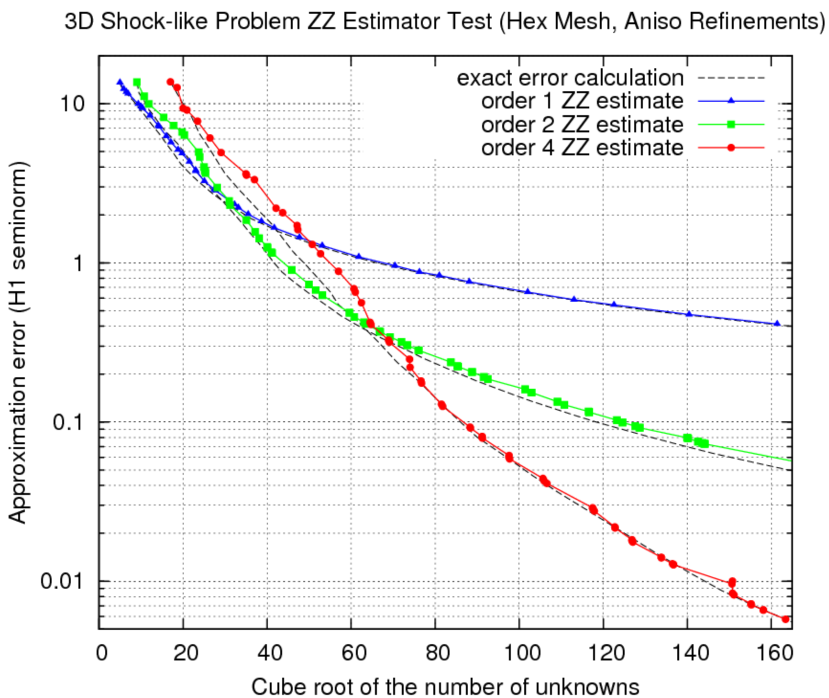
$$F = \rho \nabla u \qquad \eta_K = \|F - F_{avg}\|_{L_2(K)}$$

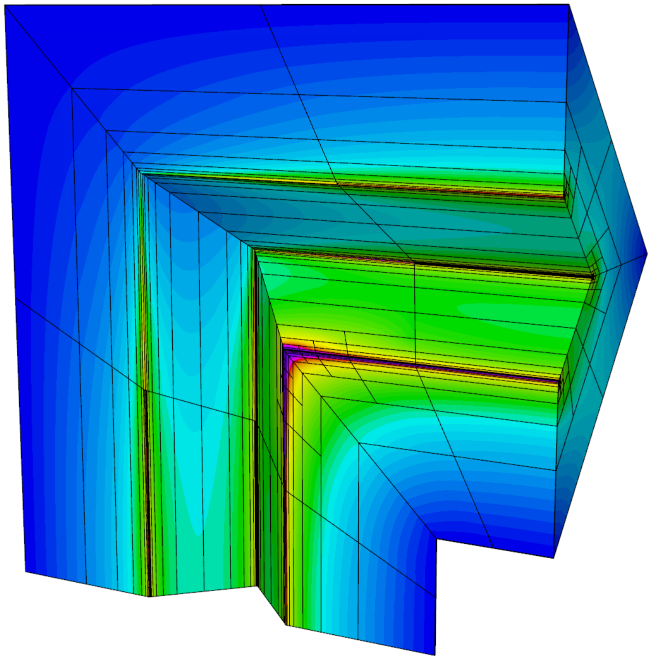
- Anisotropic version

$$(\nu_K)_{x,y,z} = \|(F - F_{avg}) \cdot J_K e_{x,y,z}\|_{L_2(K)}$$

- Simple and close to using exact error

- H(curl) EM problems can really benefit from high-order AMR
  - MFEM supports it "out of the box"
- Working on extending the anisotropic ZZ estimator to H(curl)
- Preliminary magnetostatic results:





Magnetic field magnitude in an angled pipe problem

* **mfem-3.1**, Jan 2016

H(curl) diffusion is difficult to solve

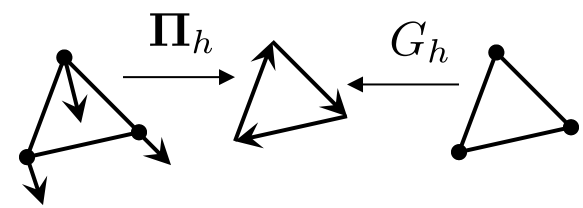
EM diffusion modeled by second order definite Maxwell

$$\nabla \times \alpha \nabla \times E + \beta E = f \quad \mapsto \quad A_h x = b$$

Challenging due to large “near-nullspace”: $\nabla \times (\nabla p_h) = 0$

Hiptmair-Xu decomposition for Nedelec elements

$$\boldsymbol{u}_h = \boldsymbol{v}_h + G_h p_h + \mathbf{\Pi}_h \boldsymbol{z}_h$$



The Auxiliary-space Maxwell Solver (AMS) achieves scalability through reduction to the nodal subspaces

$$B_h = R_h + G_h B_{v,h} G_h^t + \mathbf{\Pi}_h \boldsymbol{B}_{\boldsymbol{v},h} \mathbf{\Pi}_h^t$$

Point smoother for A_h

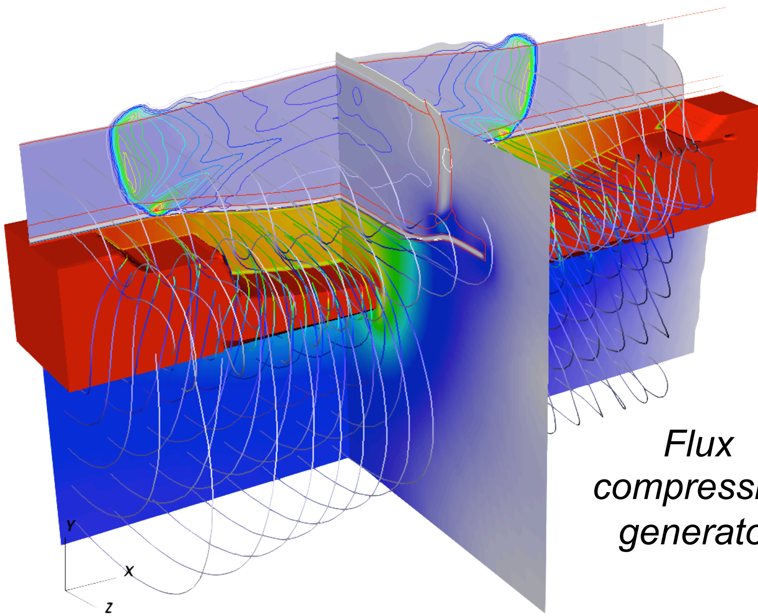
AMG solver for $G_h^t A_h G_h$

AMG solver for $\mathbf{\Pi}_h^t A_h \mathbf{\Pi}_h$

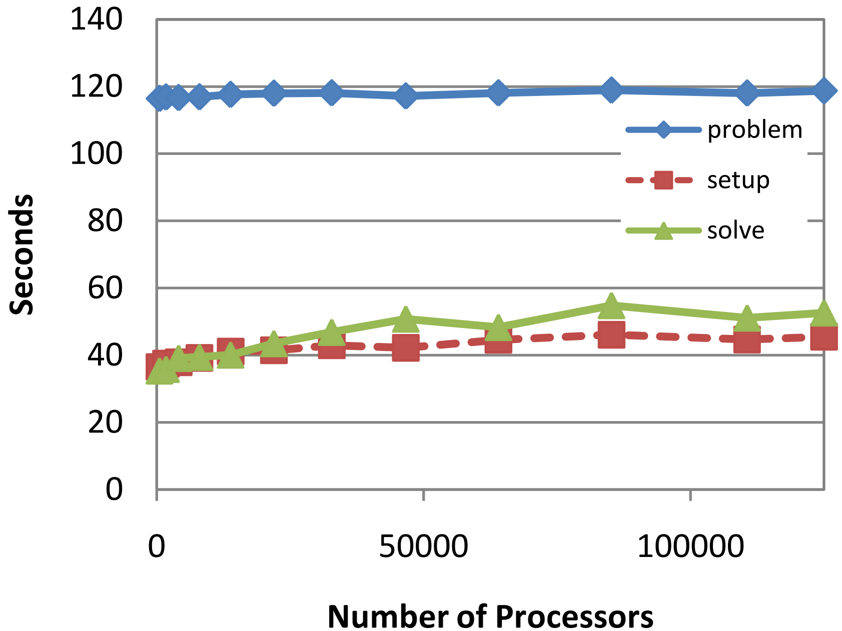
* Tz. Kolev, P. Vassilevski, **“Parallel auxiliary space AMG for H(curl) problems”**, JCM, 2009

AMS has been highly scalable for low-order discretizations on conforming meshes

AMS implementation in *hypre* requires minimal additional fine-grid information, that MFEM can generate and pass automatically.



Flux compression generator



- Significantly outperforms previous solvers ➞ up to 25x speedup
- Scaled up to 125K cores (12B unknowns)
- Solves previously intractable problems

We recently applied AMS to high-order non-conforming AMR geo-electromagnetics

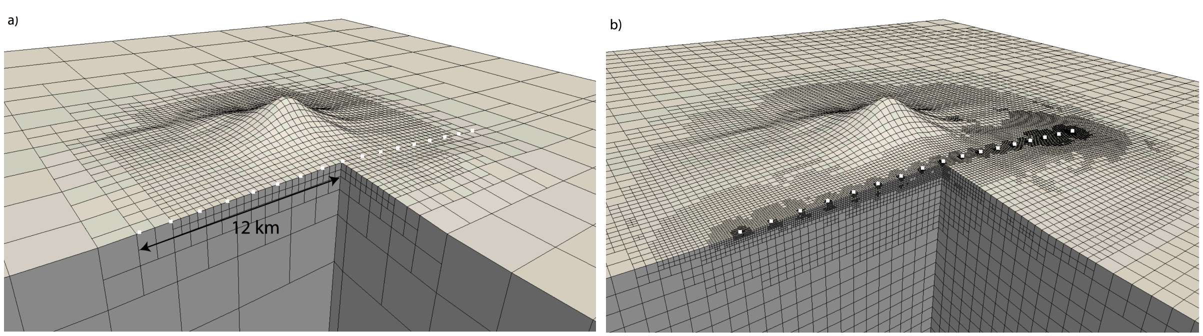
- In the high-order case, G_h and $\mathbf{\Pi}_h$ are more complicated and depend on the choice of H1 and H(curl) bases
  - MFEM has general objects to evaluate these in parallel
- Discrete gradient in the non-conforming case is defined by commutativity:

$$G_{c,h} = \mathbf{R_V} G_{nc,h} \mathbf{P}_S$$

where

$$\begin{tikzcd} S_c(\mathbb{T}) \arrow[r, "G_{c,h}"] \arrow[d, shift right, "\mathbf{P}_S"'] & \mathbf{V}_c(\mathbb{T}) \arrow[d, shift right, "\mathbf{P}_\mathbf{V}"'] \\ S_{nc}(\mathbb{T}) \arrow[r, "G_{nc,h}"] \arrow[u, shift right, "\mathbf{R}_S"'] & \mathbf{V}_{nc}(\mathbb{T}) \arrow[u, shift right, "\mathbf{R}_\mathbf{V}"'] \end{tikzcd}$$

- Magnetotelluric application $\nabla \times \alpha \nabla \times E + i\beta E$ (with A. Grayver, ETH)



2[nd] order AMR for a Kronotsky volcano model with ~12K-170K cells

Refinement step	# DoFs	N_{iter}	$\bar{N}_{iter}^{CG}$
0	647 544	22	3
6	786 436	22	3
12	2 044 156	23	3
18	9 291 488	24	4

AMS iterations ($\bar{N}_{iter}^{CG}$) for 1e-2 tolerance

* A. Grayver, Tz. Kolev, **"Large-scale 3D geo-electromagnetic modeling using parallel adaptive high-order finite element method"**, Geophysics, 2015

We are currently working on high-order radiation-diffusion and its compatible coupling with the hydro

- Multi-material single group equations (Grey diffusion)

Material energy
$$\eta_k \rho_k \frac{de_k}{dt} = \eta_k \sigma_k : \nabla v + c\eta_k \sigma_{p,k}(E - aT_k^4)$$

Radiation energy
$$\frac{dE}{dt} + \nabla \cdot \vec{F} = -c \sum_k \eta_k \sigma_{p,k}(E - aT_k^4) - E\nabla \cdot v$$

Radiation flux
$$\frac{1}{3}\nabla E = -\frac{1}{c}\sum_k \eta_k \sigma_{r,k} \vec{F}$$

$$c\mathcal{A}E - \mathcal{B}\vec{n} \cdot \vec{F} = \mathcal{C} \quad \text{on } \partial\Omega$$

- De Rham complex: H(div) fluxes match L_2 hydro thermodynamics

$$H(grad) \xrightarrow{\nabla} H(curl) \xrightarrow{\nabla \times} H(div) \xrightarrow{\nabla \cdot} L_2$$

$H(grad)$	$H(curl)$	$H(div)$	L_2
"nodes"	"edges"	"faces"	"zones"
HO kinematics	HO MHD	HO rad-diff.	HO thermodynamics

- Explicit-implicit coupling allows for generic time integration

We are currently working on high-order radiation-diffusion and its compatible coupling with the hydro

- Newton step for Backward Euler slopes:

$$\mathbf{k}^n = \mathbf{k}^{n-1} - [\partial\mathcal{N}(\mathbf{k}^{n-1})]^{-1}\mathcal{N}(\mathbf{k}^{n-1})$$

- Jacobian matrix

$$\partial\mathcal{N}(k) = \begin{bmatrix} \mathbf{M}_{\rho_\mathbf{k}} + \partial\mathbf{H}_\mathbf{k} & & -c\Delta t\mathbf{M}_{\sigma_\mathbf{k}} & 0 \\ & \ddots & \vdots & \vdots \\ -\partial\mathbf{H}_\mathbf{k} & \dots & \mathbf{M} + c\Delta t\sum_k \mathbf{M}_{\sigma_\mathbf{k}} & \mathbf{D} \\ 0 & \dots & \frac{1}{3}\Delta t\mathbf{D}^\mathbf{T} & \frac{1}{c}\mathbf{M}_\mathbf{F} + \frac{1}{3}\mathbf{B}_\mathbf{n} \end{bmatrix} \begin{bmatrix} \mathbf{k}_{\mathbf{e}_\mathbf{k}} \\ \vdots \\ \mathbf{k}_\mathbf{E} \\ \mathbf{F} \end{bmatrix}$$

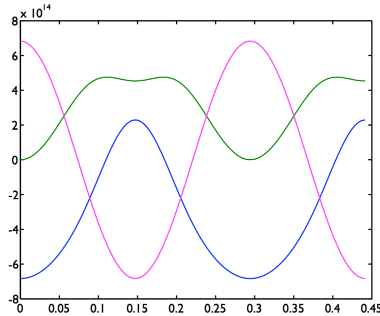
- Energies are discontinuous so their blocks can be eliminated locally
- Jacobian solve reduces to a global system for the fluxes F
- We take advantage of the scalable algebraic H(div) solver from hypre: ADS

* Tz. Kolev, P. Vassilevski, **"Parallel auxiliary space AMG for H(div) problems"**, SISC, 2012

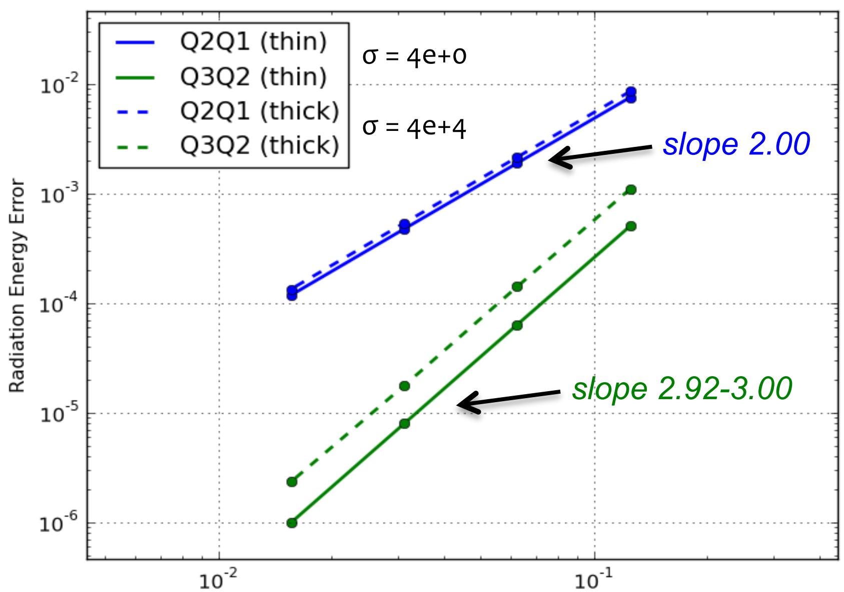
Initial coupled high-order radiation-hydrodynamics in BLAST: convergence, "crooked pipe"

$$T_{mat}(r,t) = T_0\left(1 - \frac{e^{-\tau t}}{2}\cos(\omega r)\right)$$
$$E(r,t) = aT_{rad}^4\left(1 + \frac{e^{-\tau t}}{2}\cos(\omega r)\right)$$
$$T_{rad}(r,t) = T_0\left(1 + \frac{e^{-\tau t}}{2}\right)$$

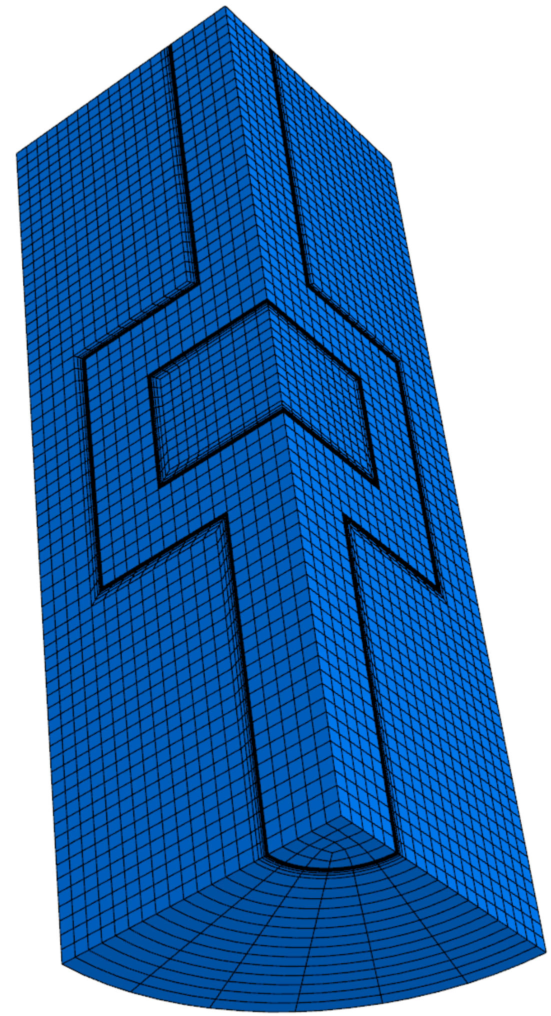
Brunner's smooth nonlinear manufactured solution



Equation terms of similar magnitudes



High-order convergence in thick & thin limits!

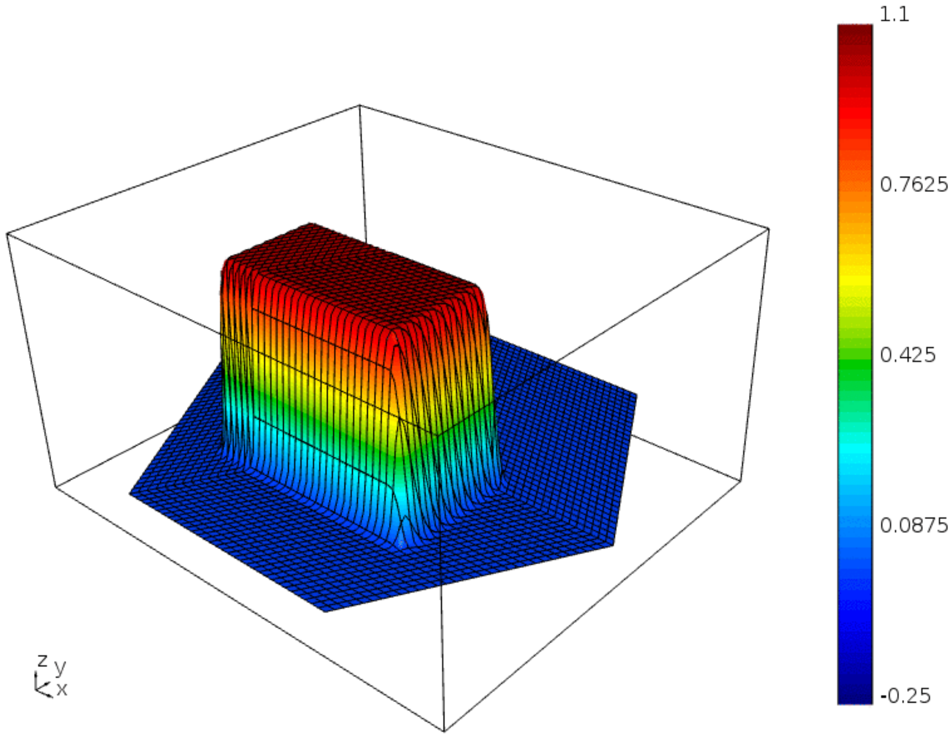


Crooked pipe, Q2-Q1 simulation

XBraid: Parallel Time Integration of High-Order Finite Element Advection-Diffusion

- 2D advection $u_t = \mathbf{b}(\mathbf{x}) \cdot \nabla u + \gamma \Delta u$
  - Periodic mesh
  - Stability determined by convection (convection dominated)
  - Diffusion term 0.001
  - Modified MFEM example targeting DG remap in BLAST

- **Sequential Time Stepping**
  - Sharp profile is transported over 1100 time steps
  - 3rd order explicit method
  - 3-level XBraid hierarchy



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- **Parallel-in-time solution**
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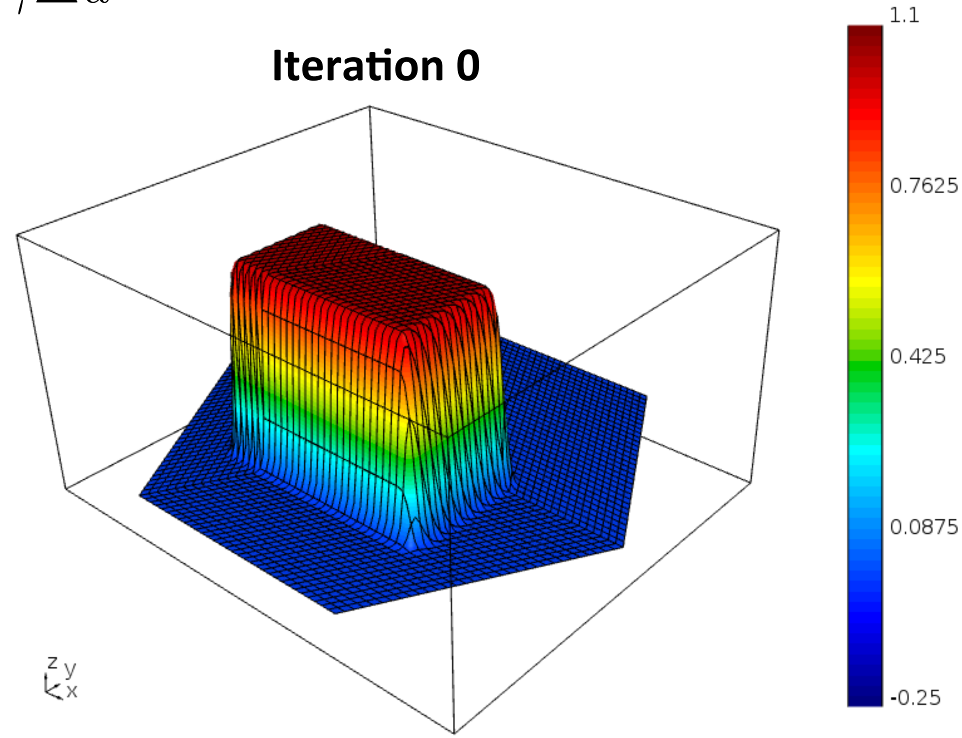
  - 3-level XBraid hierarchy

XBRAID PARALLEL MULTIGRID IN TIME

www.llnl.gov/casc/xbraid

Iteration 0



Initial guess t≥0

* R. Falgout, S. Friedhoff, Tz. Kolev, S. MacLachlan, J. Schroder **"Parallel time integration with multigrid"**, SISC, 2014

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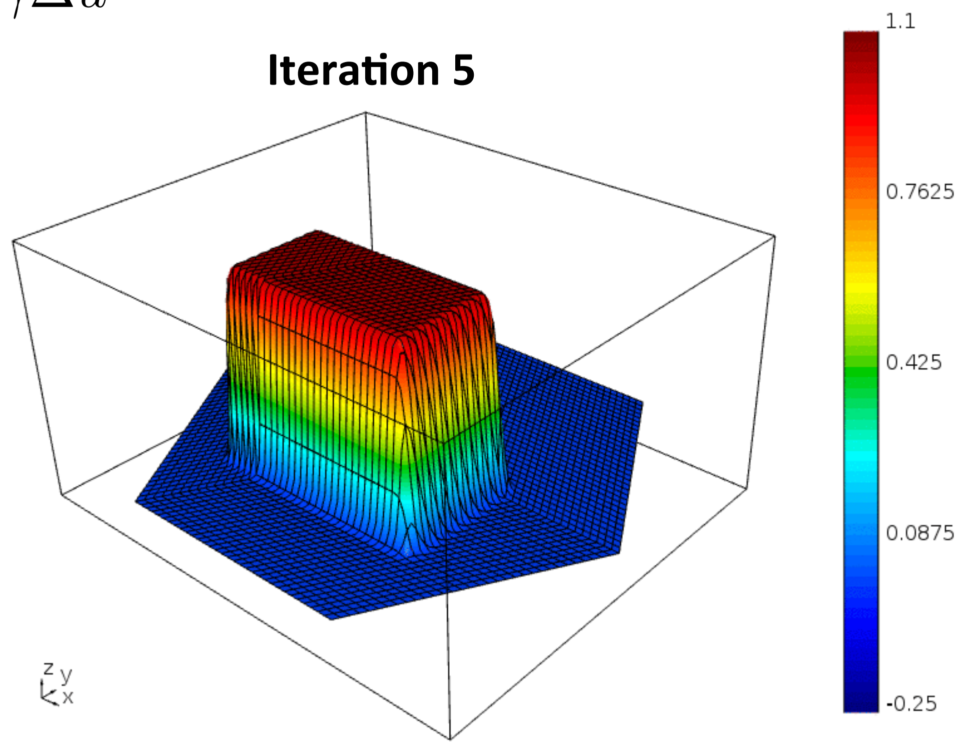

PARALLEL MULTIGRID IN TIME

www.llnl.gov/casc/xbraid

* R. Falgout, S. Friedhoff, Tz. Kolev, S. MacLachlan, J. Schroder **“Parallel time integration with multigrid”**, SISC, 2014

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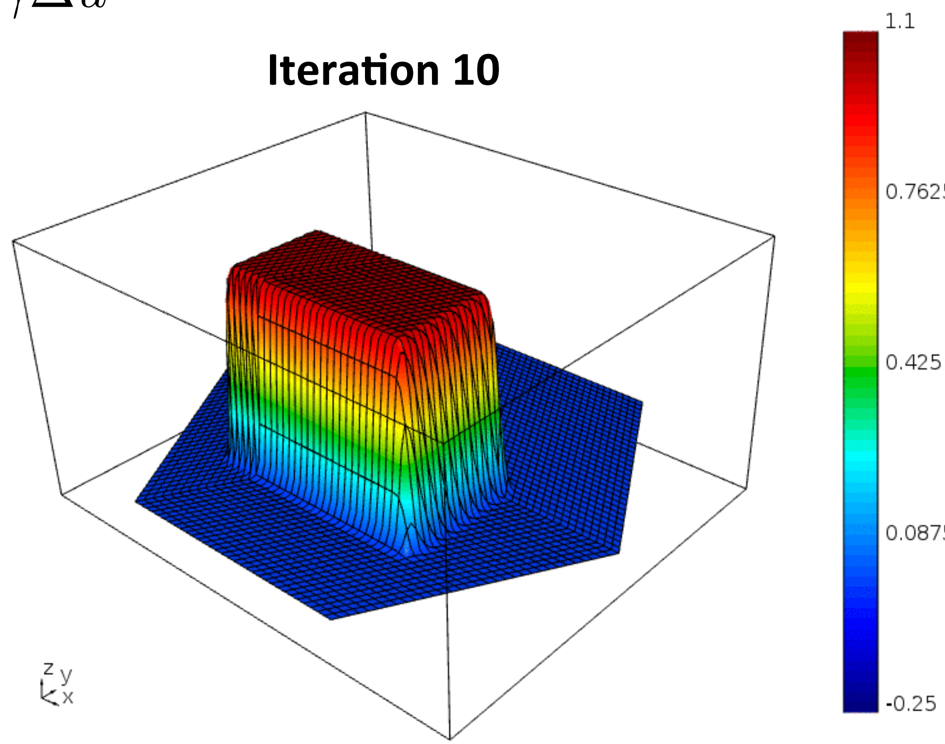


XBRAID PARALLEL MULTIGRID IN TIME

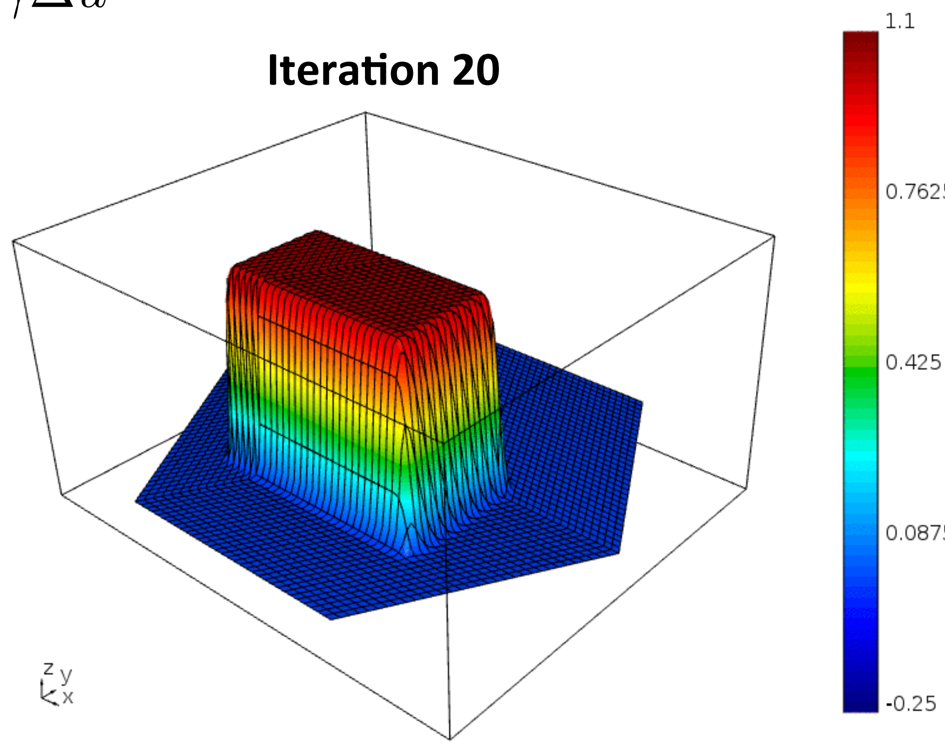
www.llnl.gov/casc/xbraid

* R. Falgout, S. Friedhoff, Tz. Kolev, S. MacLachlan, J. Schroder **"Parallel time integration with multigrid"**, SISC, 2014

XBraid: Parallel Time Integration of High-Order Finite Element Advection-Diffusion

- 2D advection $u_t = \mathbf{b}(\mathbf{x}) \cdot \nabla u + \gamma \Delta u$
  - Stability determined by convection (convection dominated)
  - Diffusion term 0.001
- **Parallel-in-time solution**
  - Sharp profile is transported over 1100 time steps
  - 3rd order explicit method
  - 3-level XBraid hierarchy
- Future Work:
  - improve convergence (relaxation, coarse-grid equations)
  - pure advection

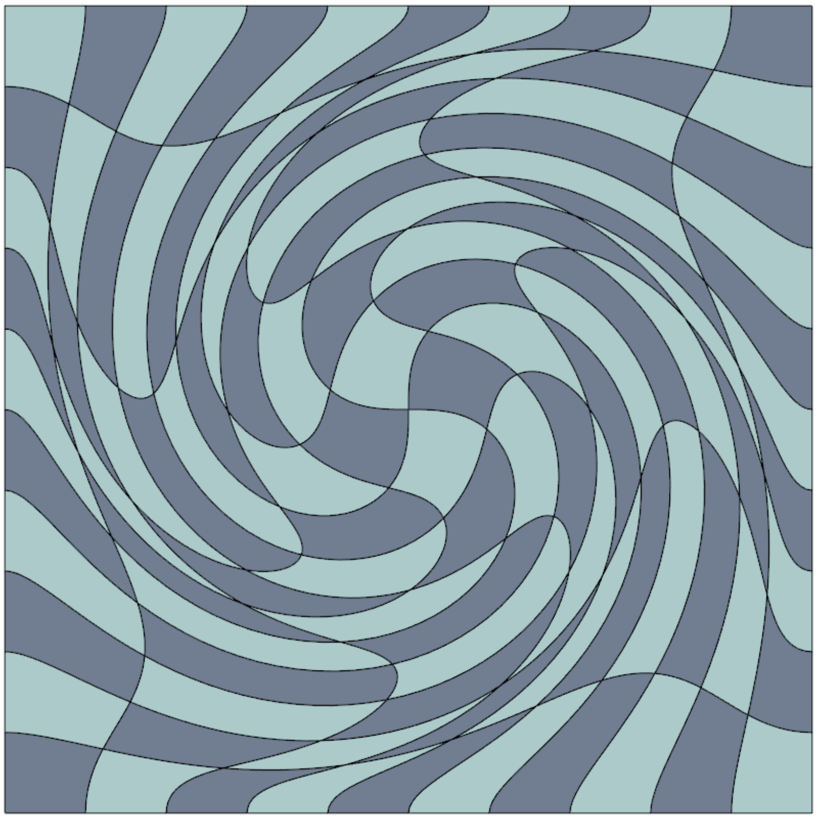
Iteration 20



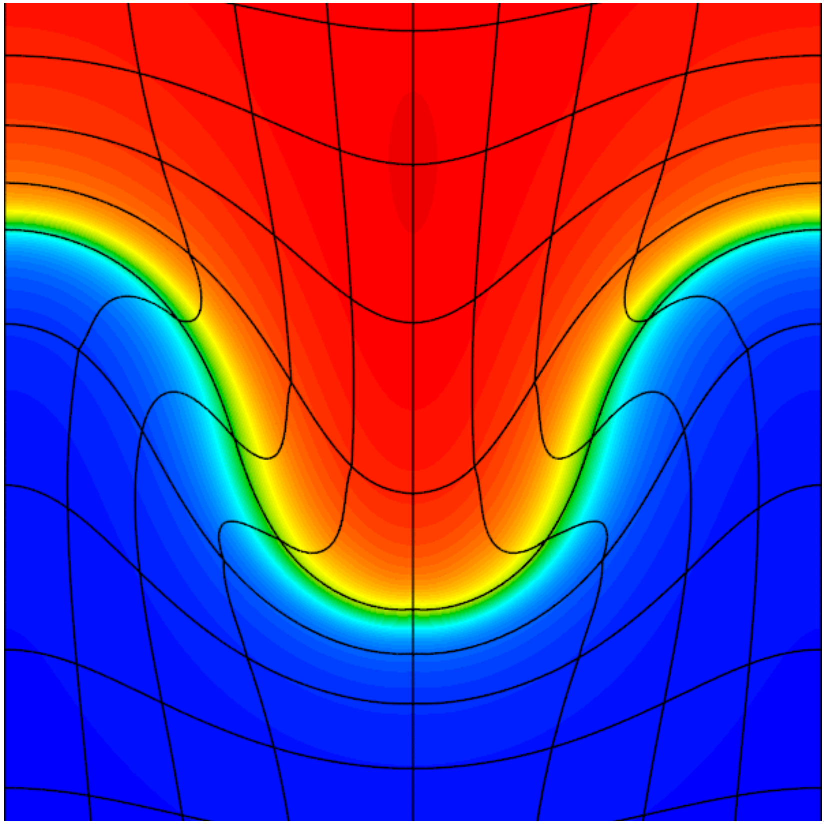
* R. Falgout, S. Friedhoff, Tz. Kolev, S. MacLachlan, J. Schroder **"Parallel time integration with multigrid"**, SISC, 2014

We are developing general tools for HO mesh optimization and high-quality interpolation between meshes

We target *high-order curved elements* + *unstructured meshes* + *moving meshes*



High-order mesh relaxation in MFEM (neo-Hookean evolution)

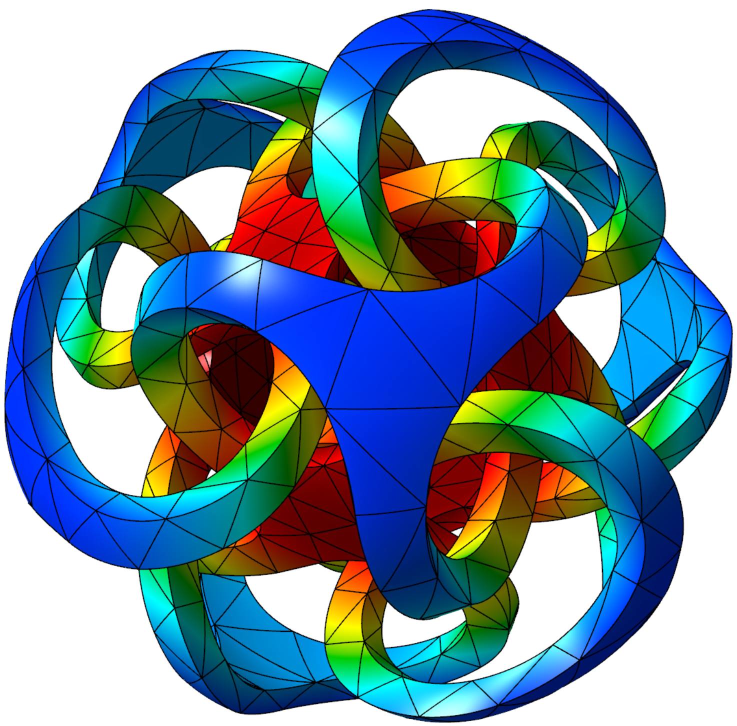


Advection-based interpolation (DG pseudo-time remap in BLAST)

We are developing general tools for accurate and flexible finite element visualization

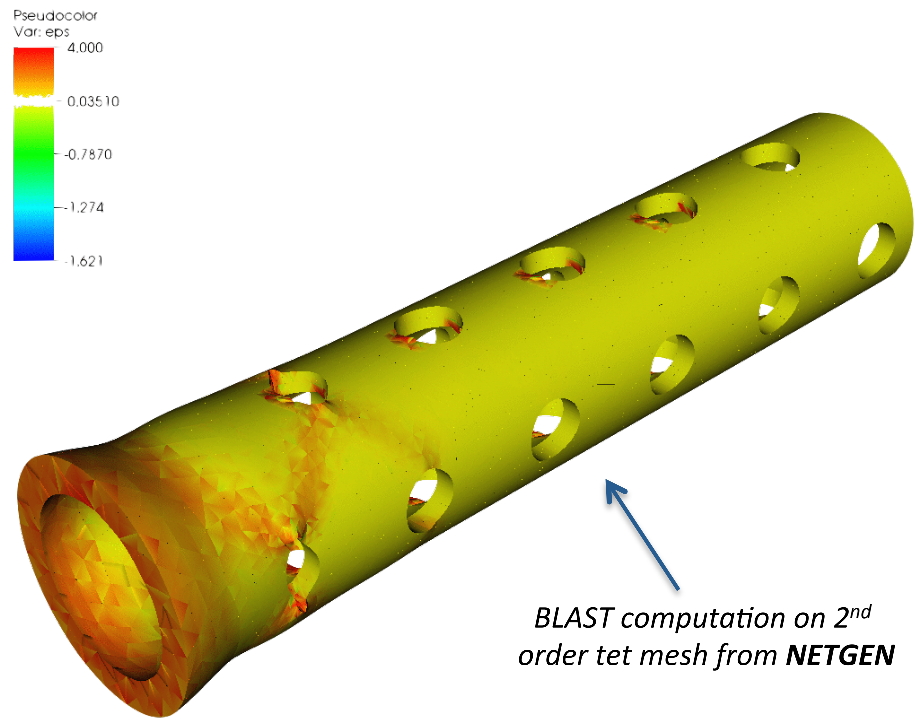
Two visualization options for high-order functions on high-order meshes.

GLVis: *native MFEM lightweight OpenGL visualization tool*



glvis.org

VisIt: *general data analysis tool, MFEM support since version 2.9*

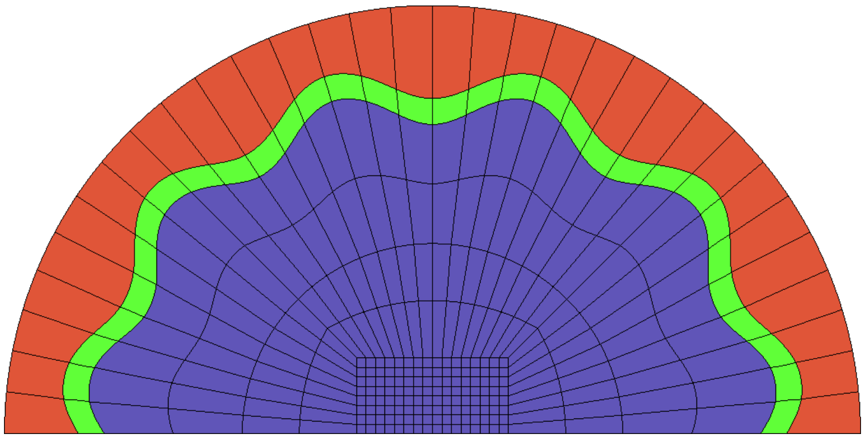


BLAST computation on 2nd order tet mesh from ***NETGEN***

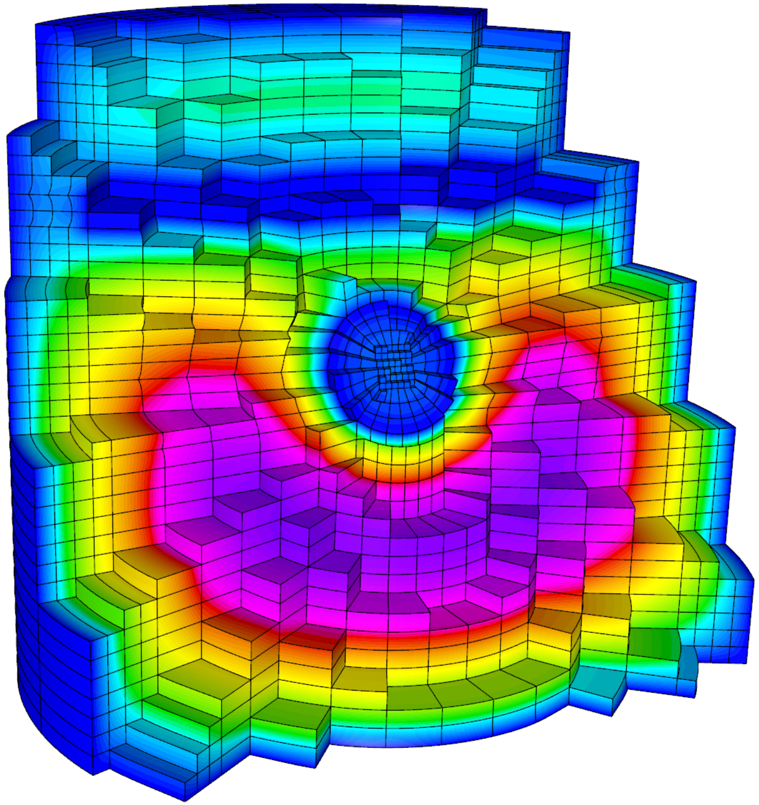
visit.llnl.gov

NURBS support in MFEM allows for accurate geometry description with relatively coarse meshes

NURBS meshes generated by the PMESH project at LLNL

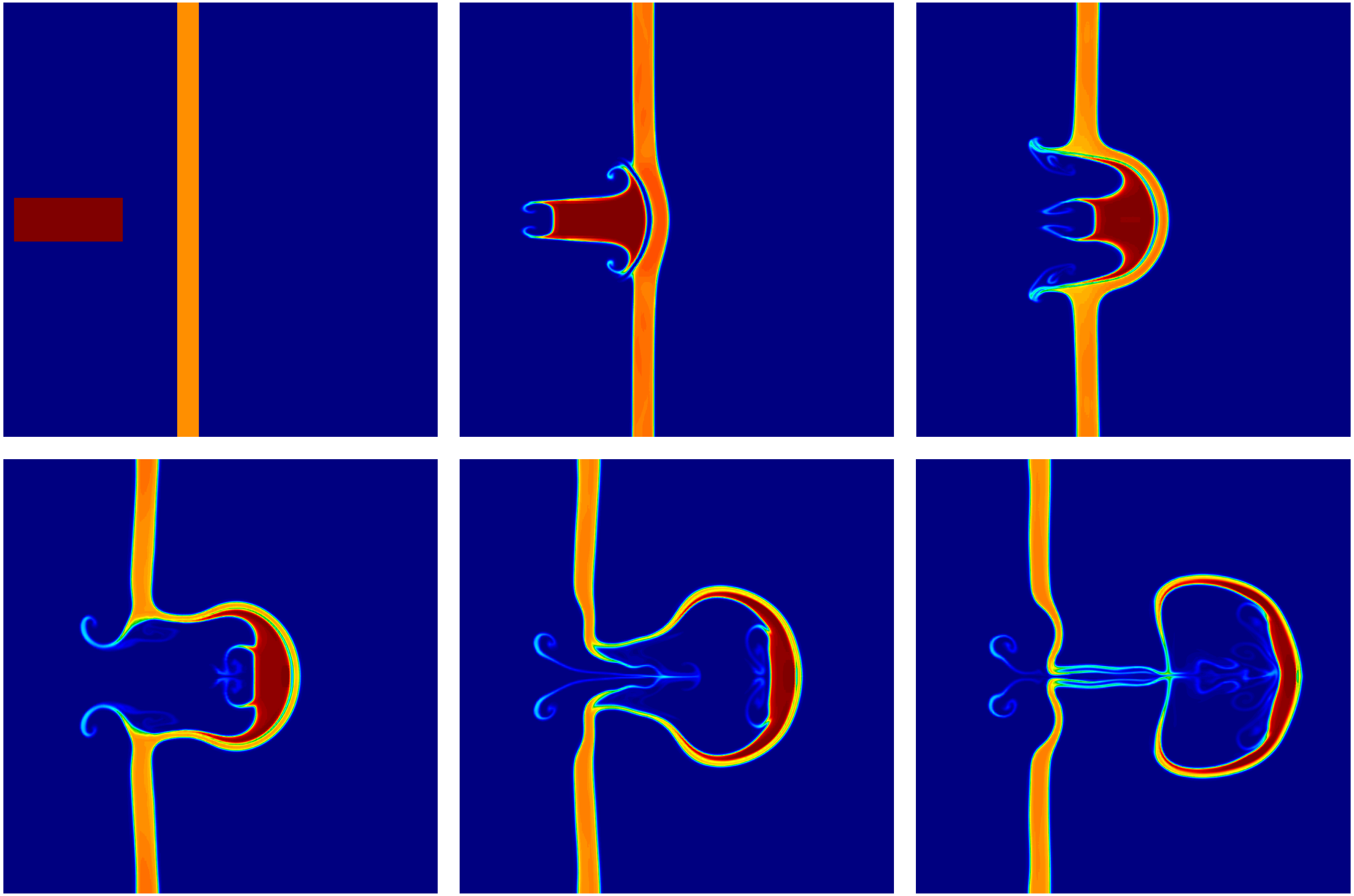


2D mesh with 3 material attributes; the interface is represented exactly



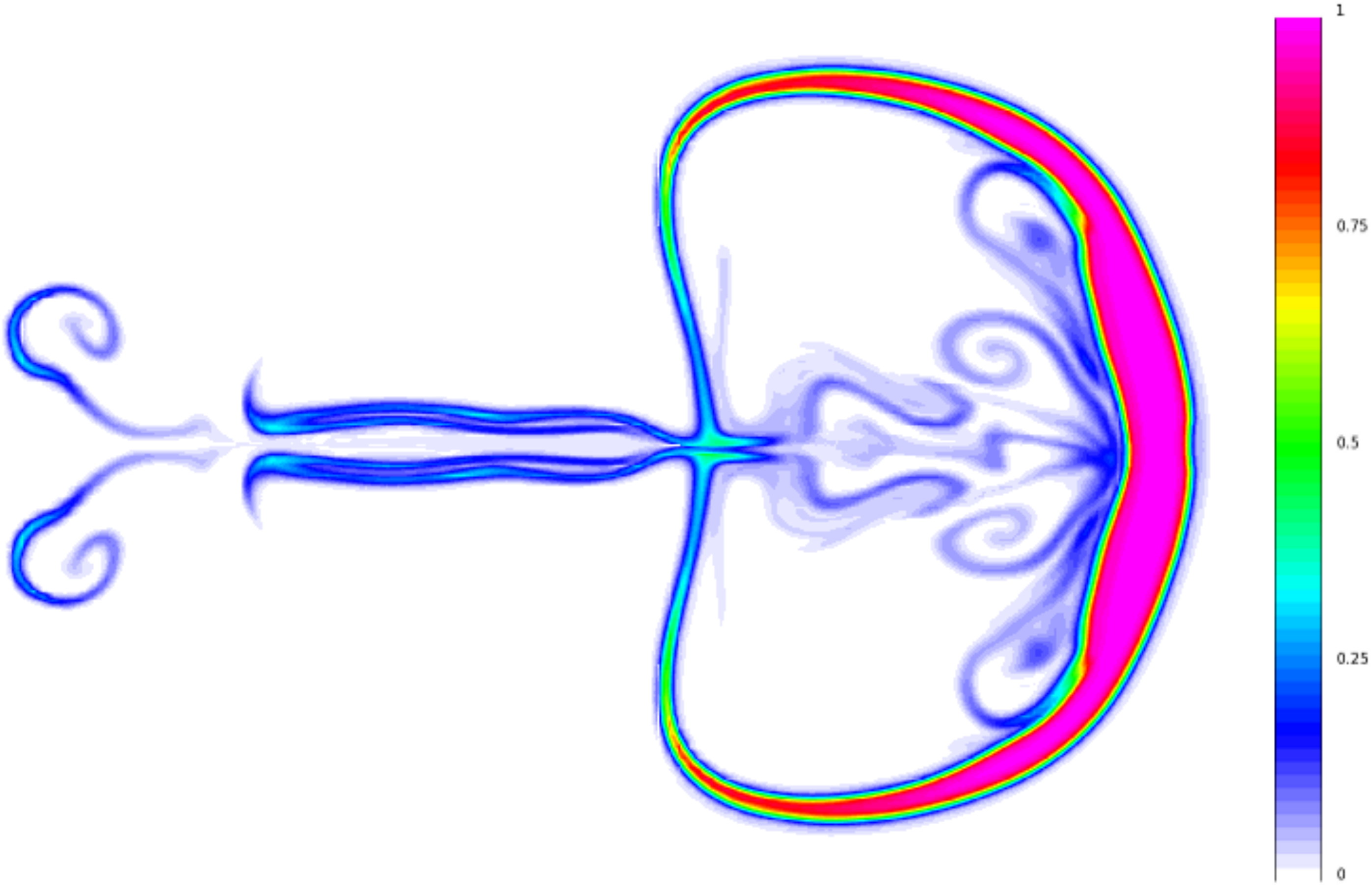
FEM solution of the Laplace equation on a 3D NURBS mesh

High-order closure model essential for problems with vastly different materials



Total density profile of gas impact test at times t=0, 2, 4, 6, 8 and 10

Closure model enables high-resolution material representation without interface reconstruction



Material indicator function of the gas impactor at final time

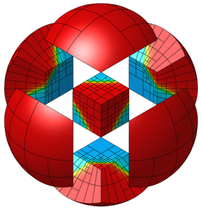
* V. Tomov et al., **"Multi-Material closure models for high-order finite element Lagrangian hydrodynamics"**, in preparation

Current and future work

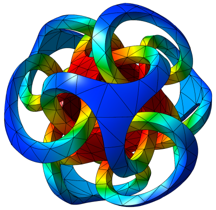
- High-order finite elements show promise for scalable multi-physics ALE simulations
- Some ongoing research:
  - improve artificial viscosity, closure model and monotonicity methods
  - port and optimize our software stack for upcoming architectures
  - extend AMR to parallel DG and load balancing
  - develop solvers for partially assembled operators
  - parallelize in time (XBraid project)
- Papers and additional details:

  people.llnl.gov/kolev1

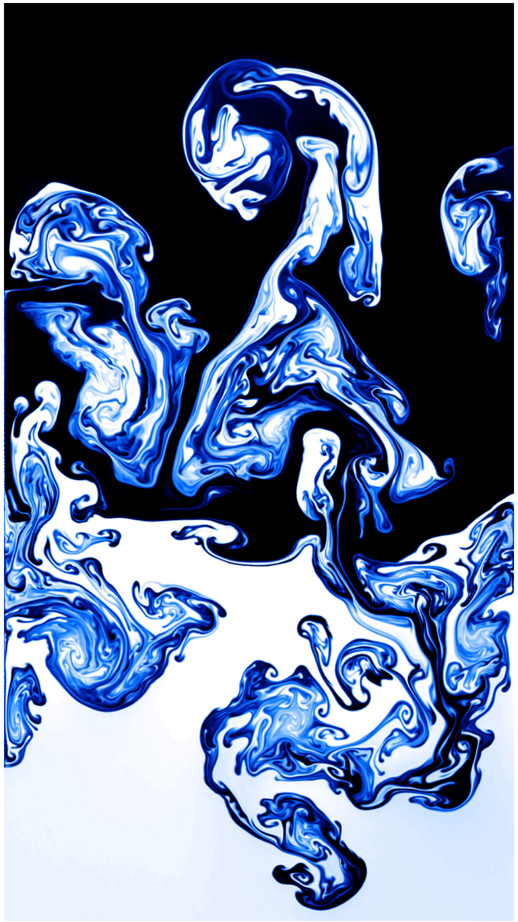
- Open-source finite element software:



mfem.org



glvis.org



Q4 Rayleigh-Taylor single-material ALE on 256 processors