Radiation Hydrodynamics with High-Order Finite Elements in the BLAST Code

MultiMat 2017, Santa Fe

Vladimir Tomov
R. Anderson, T. Brunner, V. Dobrev, Tz. Kolev, and R. Rieben

September 20, 2017

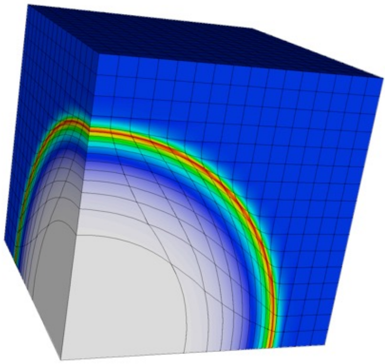
LLNL-PRES-734705
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

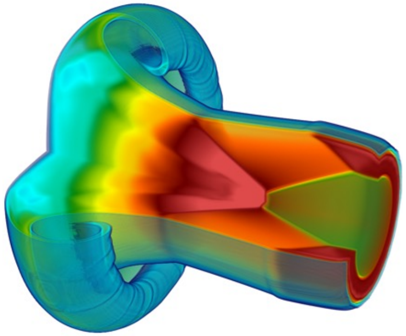
Lawrence Livermore National Laboratory

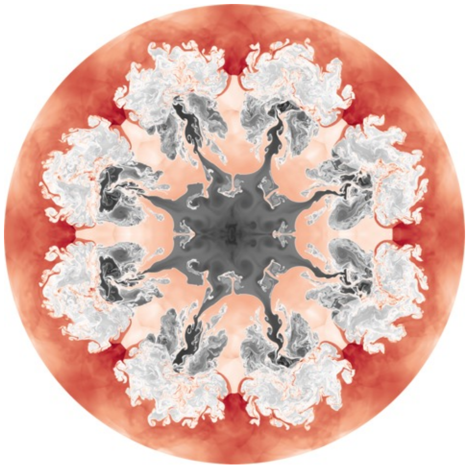
BLAST is a high-order finite element ALE code

We solve the Euler equations by a Lagrange + remap method

- Multi-material support for general EOS, strength and elasto-plastic flow models.
- Support for 2Dxy, 2Drz and 3D curved tri/tet/quad/hex meshes.
- Robustness and symmetry, reduction of mesh imprinting.
- High-order convergence on smooth tests for the full ALE algorithm.
- FLOP-intensive numerical kernels.
- Coupled to single-group rad-diffusion, MHD coupling is in progress.







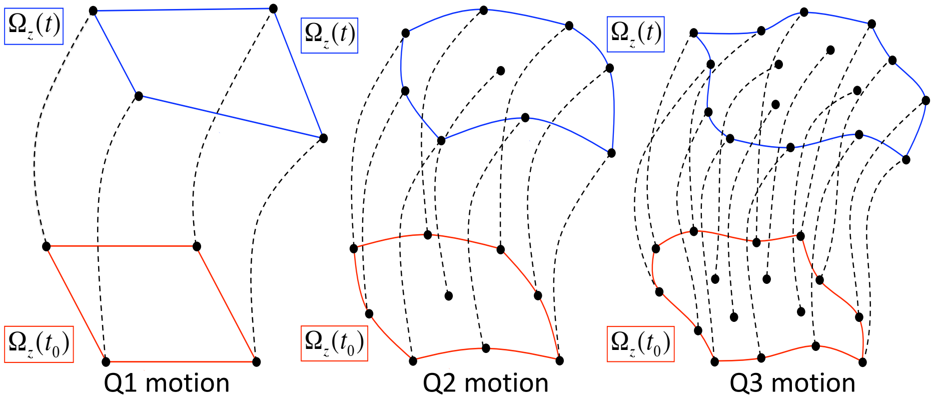
Multi-material Lagrangian phase overview

Sub-zonal resolution by combining H^1, L_2, and point-wise quantities

$$\frac{d\eta_k}{dt} = \alpha_k, \quad \frac{d(\eta_k \rho_k)}{dt} = -\eta_k \rho_k \nabla \cdot v$$

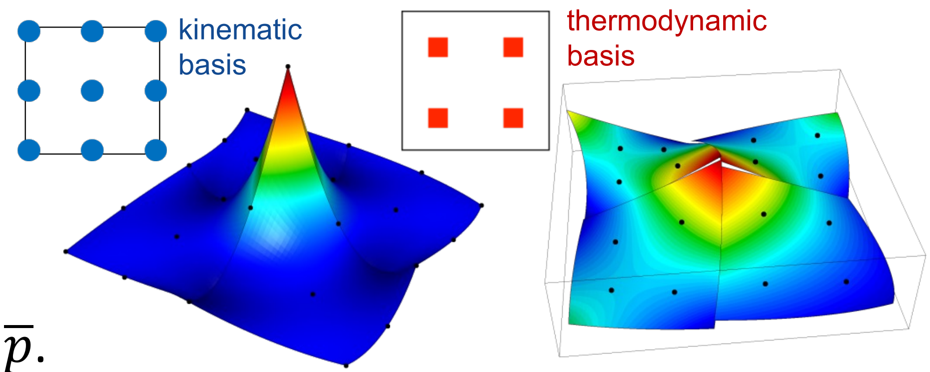
$$\frac{dx}{dt} = v, \quad \sum_k \eta_k \rho_k \frac{dv}{dt} = \nabla \cdot \sum_k \eta_k \sigma_k$$

$$\eta_k \rho_k \frac{de_k}{dt} = \eta_k \sigma_k : \nabla v - \alpha_k \bar{p}$$



Curvilinear zones represent material flow better

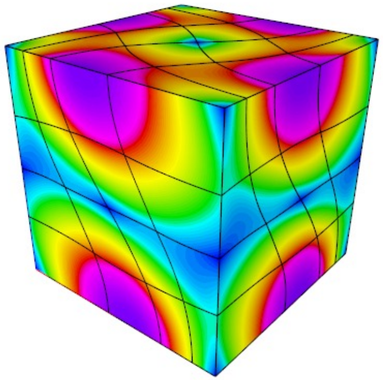
- Continuous HO kinematics for position x, velocity v.
- Discontinuous HO thermodynamics for specific internal energies e_k.
- Point-wise closure computations for volume fractions η_k, increments α_k and $\bar{p}$.
- Point-wise mass conservation for densities ρ_k.

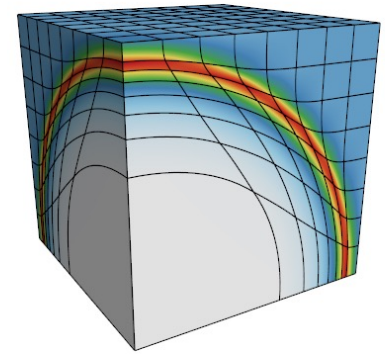


High-order fields lead to sub-zonal resolution

LAGHOS: LAGrangian High-Order Solver

Laghos is a new MFEM miniapp for high order hydrodynamics





- Public GitHub website: https://github.com/CEED/Laghos
  - Email list: laghos@llnl.gov
- Resembles the single material Lagrangian phase of BLAST.
- Supports full assembly and partial assembly options.
- Supports 2D and 3D unstructured meshes - quads / hexes, triangles / tets.
- C++ code with domain-decomposed MPI parallelism.
- Optional in-situ visualization with GLVis.

High-order mesh optimization phase overview

Based on node movement that is controlled by the TMOP paradigm

- We extend the Target-Matrix Optimization Paradigm (TMOP) to high-order meshes.
  - P. Knupp's rigorous theory is used to define high-order mesh quality.
  - Quality metrics are defined with respect to shape / size / alignment.
  - Metrics are computed on quadrature point level.

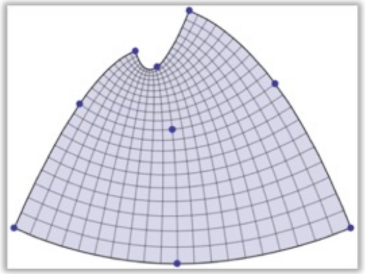
- We define a global variational minimization problem to find the optimal node positions:

$$F(x) = \sum_K \int_K \mu(x); \qquad \frac{\partial F(x)}{\partial x} = 0$$

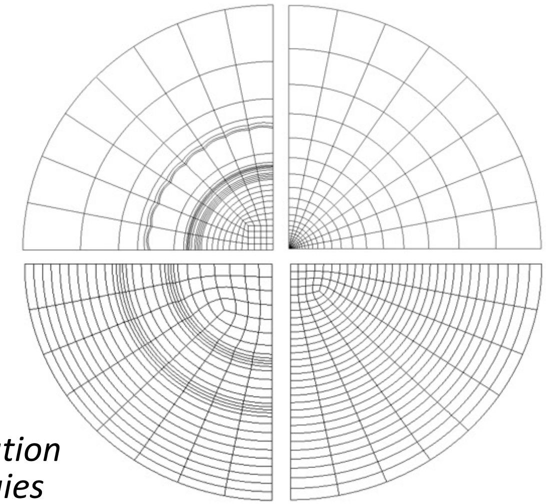
- Nonlinear solver is applied to the resulting system.

- Capabilities include for compositions of metrics, limited movement, space-time coefficients.

ethos



Example of a Q_2 zone



Example of optimization by different strategies

Remap phase overview

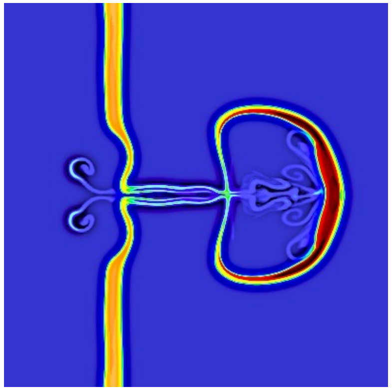
Conserved fields are evolved by a sequential FCT algorithm

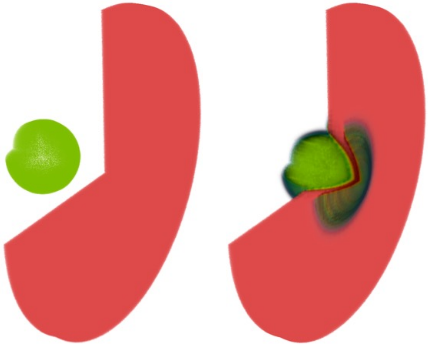
$$\frac{dx}{d\tau} = u \qquad \frac{d\eta}{d\tau} = u \cdot \nabla \eta$$
$$x(0) = x_0 \qquad \eta(x,0) = \eta_0(x)$$

- Formulated as pseudo-time advection.
- We remap (solve for) momentum, volumes, masses, internal energies.
  - Conserved on semi-discrete level.
  - Monotone and conservative transitions to these new variables.
- Bounds are preserved for the primal variables:

$$\eta_{k,i}^{\min} \le \eta_{k,i}^{n+1} \le \eta_{k,i}^{\max}, \quad \rho_{k,i}^{\min} \le \frac{(\eta\rho)_{k,i}^{n+1}}{\eta_{k,i}^{n+1}} \le \rho_{k,i}^{\max}, \quad e_{k,i}^{\min} \le \frac{(\eta\rho e)_{k,i}^{n+1}}{(\eta\rho)_{k,i}^{n+1}} \le e_{k,i}^{\max}$$

- Monotonicity is achieved by a sequential FCT method.
  - Compute η_k → compute $(\eta\rho)_k$ → compute $(\eta\rho e)_k$





V. Dobrev, Tz. Kolev, R. Rieben, "High-order curvilinear finite element methods for Lagrangian hydrodynamics", SIAM J. Sci. Comp., 34(5):604–641, 2012.
V. Dobrev, Tz. Kolev, R. Rieben, V. Tomov, "Multi-material closure model for high-order finite element Lagrangian hydrodynamics", IJNMF, 82(10):689-706, 2016.
R. Anderson, V. Dobrev, Tz. Kolev, R. Rieben, V. Tomov, "High-order multi-material ALE hydrodynamics", Under Review, 2017.

Coupling to grey radiation diffusion

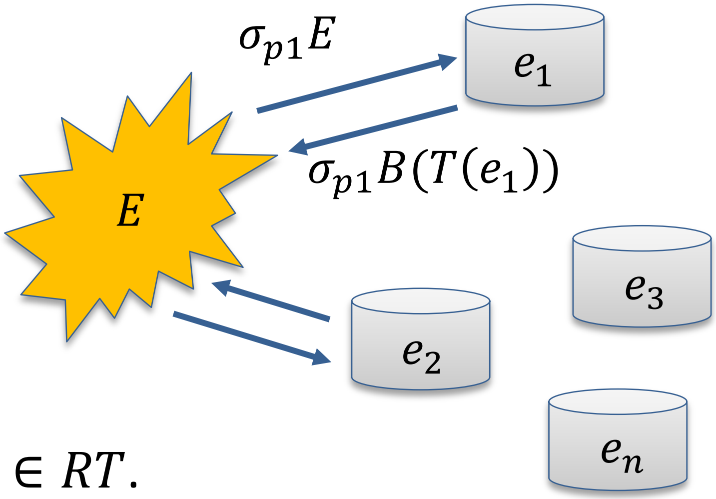
We utilize the $H(div)$ flux formulation

$$\eta_k \rho_k \frac{\partial e_k}{\partial t} = \eta_k \sigma_k : \nabla v - \alpha_k \bar{p} + \eta_k \; c \; \sigma_{p,k} \big(E - B(T(e_k)) \big) \, ,$$

$$\frac{\partial E}{\partial t} + \nabla \cdot F = - \sum_k \big(\eta_k \; c \; \sigma_{p,k} \left(E - B(T(e_k)) \right) \big) \, ,$$

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

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



- Avoiding DG jump terms, we choose $\mathrm{E} \in L_2, F \in RT$.

$H(grad)$ "nodes" $\xrightarrow{\nabla}$ $H(curl)$ "edges" $\xrightarrow{\nabla\times}$ $H(div)$ "faces" $\xrightarrow{\nabla\cdot}$ L_2 "zones"

HO kinematics — HO MHD — HO rad-diff. — HO thermodynamics

- Implicit treatment for e_k and E, leading to a non-linear system.
- The hydro terms are explicit, and we lag opacities.
- General EOS and temperature-dependent opacity model for each material.

Fully-discrete discretization details

The problem is reduced to inverting a Jacobian system

- General implicit time step: $k = \mathcal{F}(y^n + \Delta t k)\,; k = (\dots k_{e_k} \dots, k_E)$
- Semi-discrete system: $\mathcal{N}(k) = 0$

$$\mathcal{N}(k) = \begin{pmatrix} L_{\rho_k} k_{e_k} + H_k(k_{e_k}) - c\Delta t L_{\sigma_k} k_E - h_k + c L_{\sigma_k} E \\ -\sum_k H_k(k_{e_k}) + L k_E + c\Delta t \sum_k L_{\sigma_k} k_E + DF - c \sum_k L_{\sigma_k} E \\ \frac{1}{3}\Delta t D^T k_E + \frac{1}{c} R_\sigma F + \frac{1}{3} R_n F + \frac{1}{3} b_n - \frac{1}{3} D^T E \end{pmatrix}$$

L matrices are local L_2
R matrices are global RT
D matrix is transition $L_2 - RT$
H is non-linear operator on L_2

- We use Newton's method to solve the resulting non-linear system:

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

- The Jacobian matrix of the grey diffusion approximation has this form:

$$\partial \mathcal{N}(k) = \begin{bmatrix} \ddots & & \mathbf{0} & \vdots & \vdots \\ & L_{\rho_k} + \partial H_k & & -c\Delta t L_{\sigma_k} & 0 \\ \mathbf{0} & & \ddots & \vdots & \vdots \\ \dots & -\partial H_k & \dots & L + c\Delta t \sum_k L_{\sigma_k} & D \\ \dots & 0 & \dots & \frac{1}{3}\Delta t D^T & \frac{1}{c} R_\sigma + \frac{1}{3} R_n \end{bmatrix}$$

Material energies
Rad energy
Rad flux

Approach #1: inverting the Jacobian matrix

Reduces to a global $H(div)$ linear system and local L_2 problems

$$\partial\mathcal{N}(k) = \begin{bmatrix} \ddots & & \mathbf{0} & \vdots & \vdots \\ & L_{\rho_k} + \partial H_k & & -c\Delta t L_{\sigma_k} & 0 \\ \mathbf{0} & & \ddots & \vdots & \vdots \\ \dots & -\partial H_k & \dots & L + c\Delta t \sum_k L_{\sigma_k} & D \\ \dots & 0 & \dots & \frac{1}{3}\Delta t D^T & \frac{1}{c}R_\sigma + \frac{1}{3}R_n \end{bmatrix}$$

Material energies

Rad energy

Rad flux

- Approach #1:
  - Eliminate the material energy blocks (all k_{ek}) and the radiation energy k_E.
  - Solve the global $H(div)$ linear system to find F.
    Non-symmetric for general space-dependent densities and opacities:
    $$\left(\frac{1}{3}\Delta t D^T M_E D + \frac{1}{c}R_\sigma + \frac{1}{3}R_n\right) F = RHS, \quad M_E = L + c\Delta t \sum_k L_{\rho_k}(L_{\rho_k} + \partial H_k)^{-1} L_{\sigma_k}$$
  - Back-substitute to find k_E and each k_{ek} (by local L_2 inversions).

- We use algebraic hybridization for solving the resulting $H(div)$ systems.

  V. Dobrev, Tz. Kolev, C. S. Lee, V. Tomov, P. Vassilevski, "Algebraic hybridization and static condensation with application to scalable H(div) preconditioning", Under Review, 2017.

Approach #2: decomposition to overlapping blocks

The nonlinear solve resembles a block Gauss-Seidel type iteration

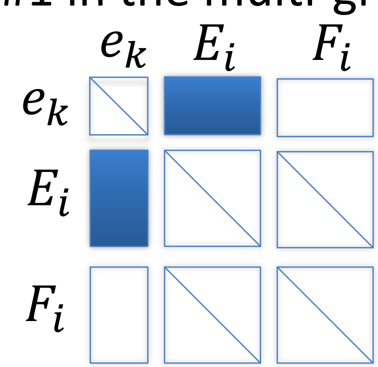
$$\partial \mathcal{N}_{energy}(k) = \begin{bmatrix} \ddots & & \mathbf{0} & \vdots \\ & L_{\rho_k} + \partial H_k & & -c\Delta t L_{\sigma_k} \\ \mathbf{0} & & \ddots & \vdots \\ \dots & -\partial H_k & \dots & L + c\Delta t \sum_k L_{\sigma_k} \end{bmatrix}$$

Material energies (first three block rows)

Rad energy (last block row)

- Approach #2 (originally proposed by P. Nowak):
  - Perform local nonlinear solves in the L_2 blocks (material and rad energies), keeping the rad flux F explicit.
  - Using the calculated k_E, solve the global $H(div)$ linear system.
- More appropriate than approach #1 in the multi-group discretization:

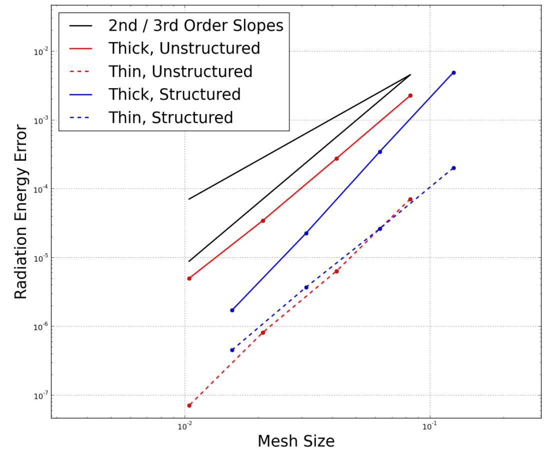
Jacobian structure for single group

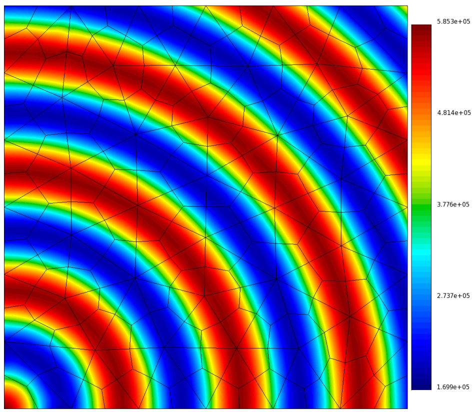


- Local coupling $e_k \leftrightarrow E_i$ (each material to each group).
- Global coupling $E_i \leftrightarrow F_i$ (groups are independent).

Smooth radiation diffusion test / Marshak wave

- Convergence on a manufactured smooth problem (Q_2/RT_2 spaces):
  - Designed so that all terms have similar magnitude.

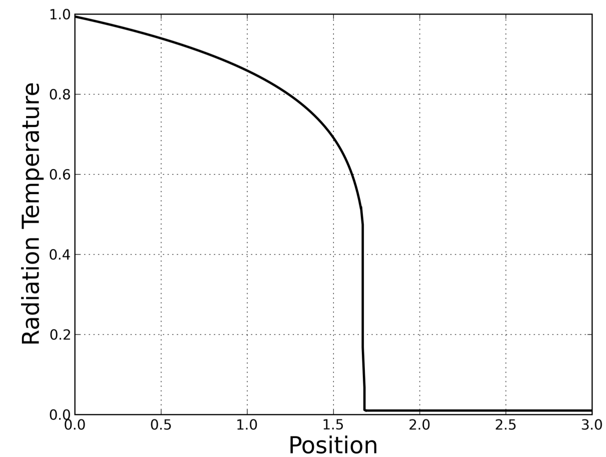




T. Brunner, “Development of a grey nonlinear thermal radiation diffusion Verification problem”, Transactions of the American Nuclear Society, 95:876-878, 2006.

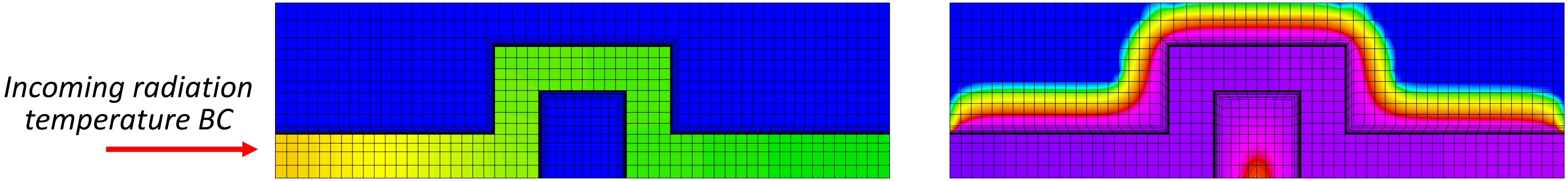
- Simulation of a Marshak-type wave:
  - Opacities are evaluated at a common continuous temperature (a high-order H^1 function).

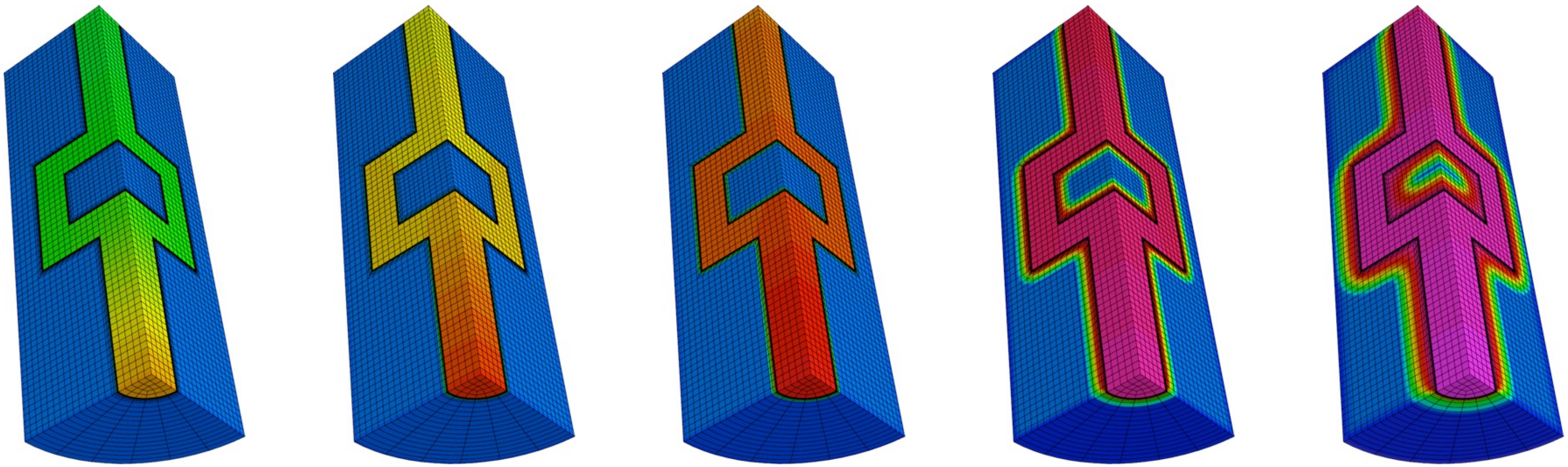
A. Irvine, I. Boyd, N. Gentile, “Reducing the spatial Discretization error of thermal emission in implicit Monte Carlo simulations”, Journal of Comp. and Theoretical Transport, 45:99-122, 2016.



The crooked pipe problem in 2Drz and 3D

- Models propagation in a low opacity region ($\sigma_a = 0.02$), surrounded by a thick ($\sigma_a = 200$) region.





Adding back the material motion

We derive a conservative 2nd order IMEX time integrator

- Material motion is altered by scattering of photons:

$$\sum_k \eta_k \rho_k \frac{dv}{dt} = \ldots + \frac{\sigma_t}{c} F, \qquad \frac{dE}{dt} = \ldots - \frac{4}{3} E \nabla \cdot v$$

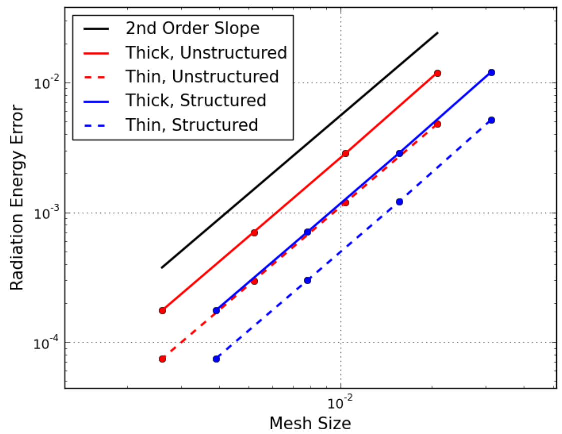
- The new terms are explicit in both equations.
  - Only the RHS of the nonlinear system is affected.

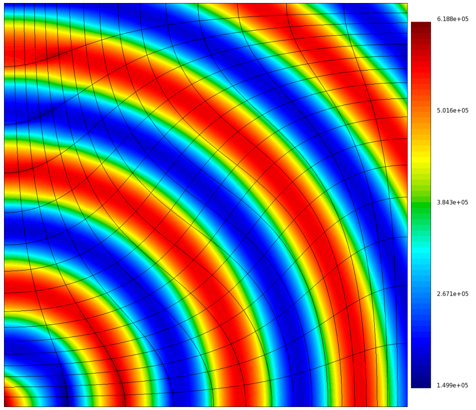
- IMEX time integrator is used to mix the velocity and energy updates.
  - Conservative 2-stage predictor-corrector method.
  - Hydro terms are evolved by a modified RK2-type of step.
  - Implicit terms are handled by backward Euler and Crank-Nicolson steps.
  - Evolves the moments of the radiation energy (time-dependent mass matrix).

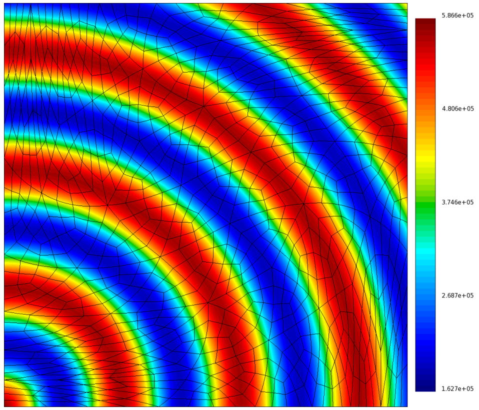
$$\int_{x^{n+1}} E^{n+1}\phi = \int_{x^n} E^n \phi - \Delta t \int_{x^{n+\frac{1}{2}}} \frac{1}{3} E^{n+\frac{1}{2}} \nabla \cdot \bar{v}^{n+\frac{1}{2}} \phi$$
$$+ \frac{\Delta t}{2} \int_{x^n} \left(-c\sigma^n (E^n - B(T^n)) - \nabla \cdot F^n\right) \phi + \frac{\Delta t}{2} \int_{x^{n+1}} \left(-c\sigma^{n+1} (E^{n+1} - B(T^{n+1})) - \nabla \cdot F^{n+1}\right) \phi$$

Smooth rad-hydro test / Lowrie shock tube

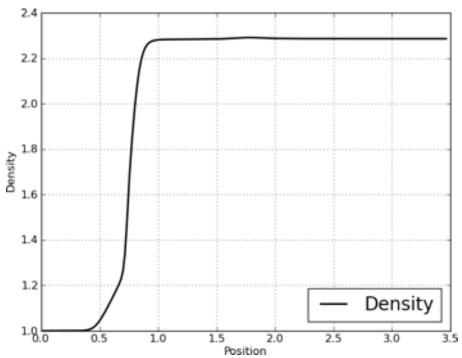
- Combination of the Taylor-Green vortex and Brunner's smooth diffusion test:
  - Analytic sources keep the manufactured solution constant in time while the mesh evolves.

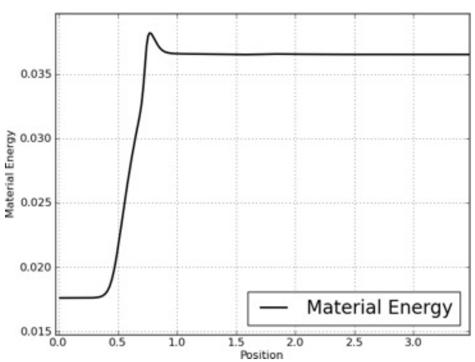


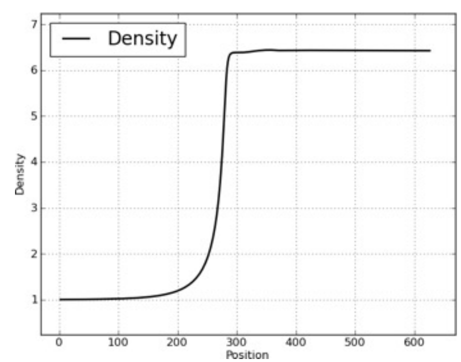


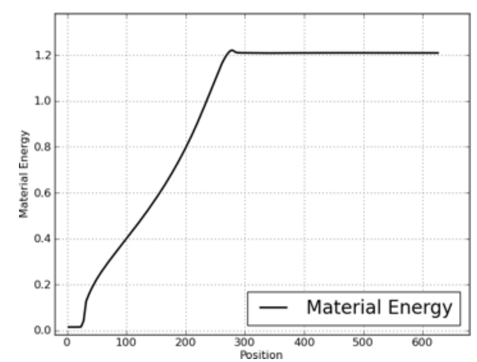


- Lowrie shock tube with temperature-dependent opacities, Mach 2 and 45:



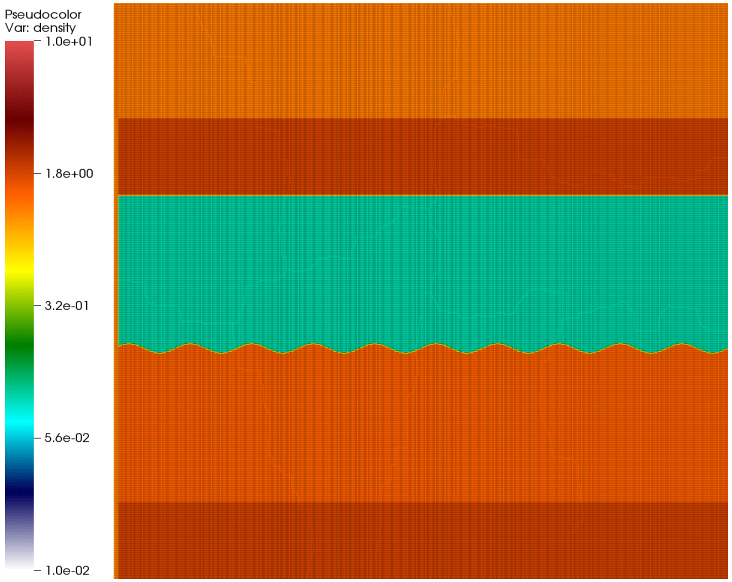


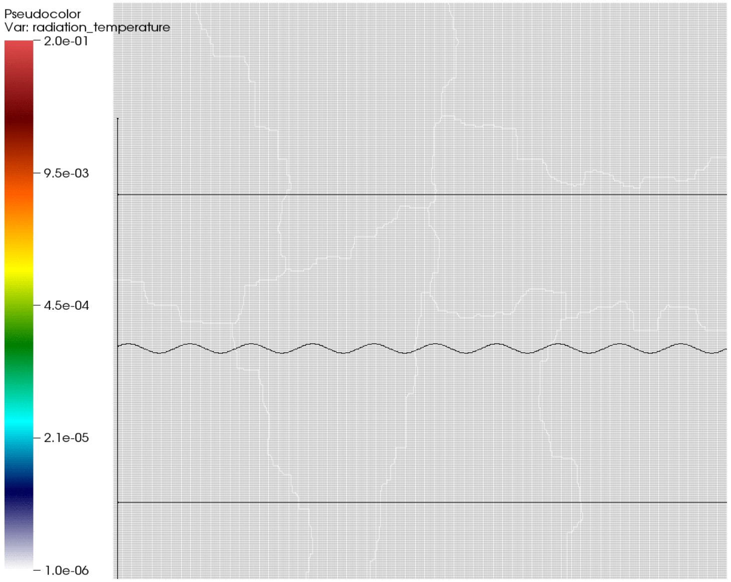




Extension to full ALE radiation hydrodynamics

- We simply remap E as a conservative variable (by the FCT advection).
  - There is no need for synchronization with the hydro variables.
  - The radiation flux F is recomputed from the result of the remap.
- Example: radiating Kelvin-Helmholtz instability:
  - 5 materials (ideal gases), Q_2Q_1 discretization, constant opacities.

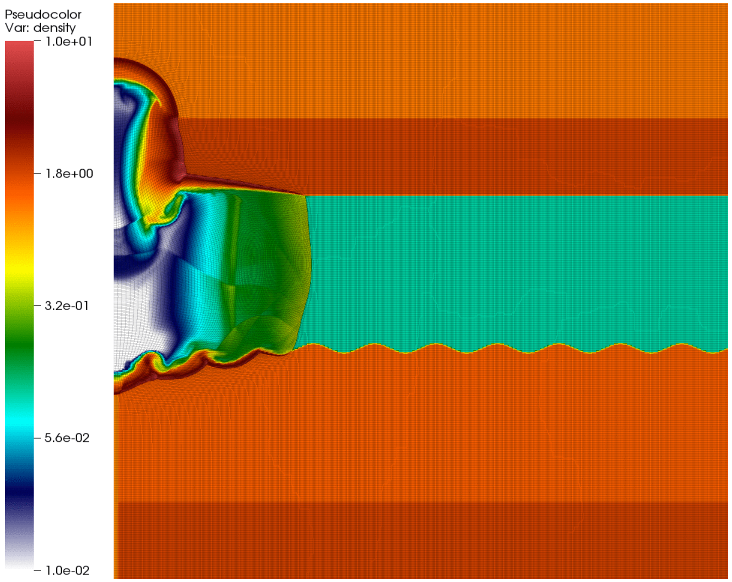


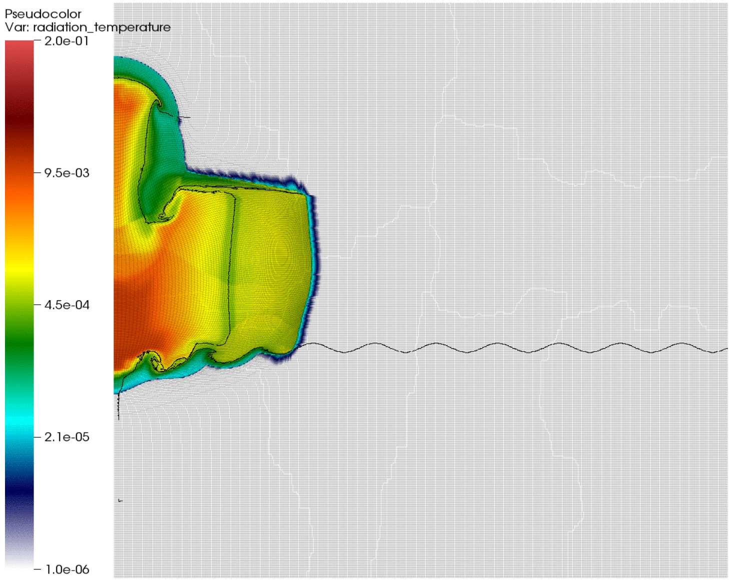


Extension to full ALE radiation hydrodynamics

- We simply remap E as a conservative variable (by the FCT advection).
  - There is no need for synchronization with the hydro variables.
  - The radiation flux F is recomputed from the result of the remap.

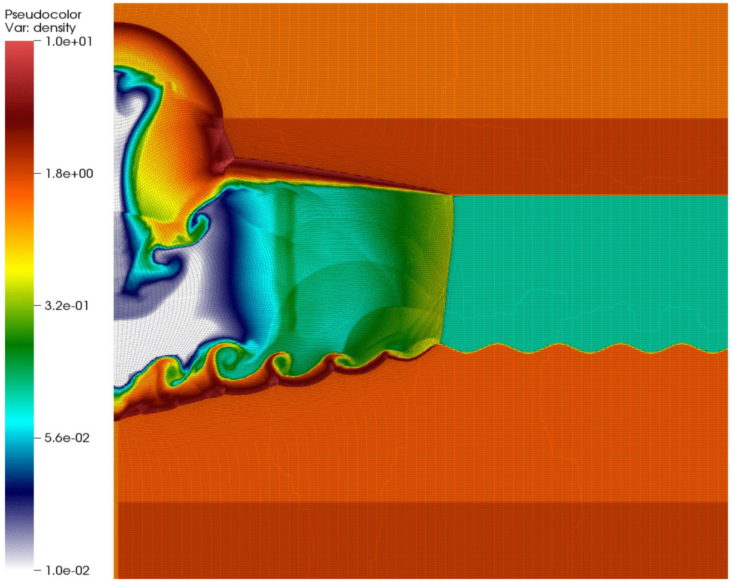
- Example: radiating Kelvin-Helmholtz instability:
  - 5 materials (ideal gases), Q_2Q_1 discretization, constant opacities.

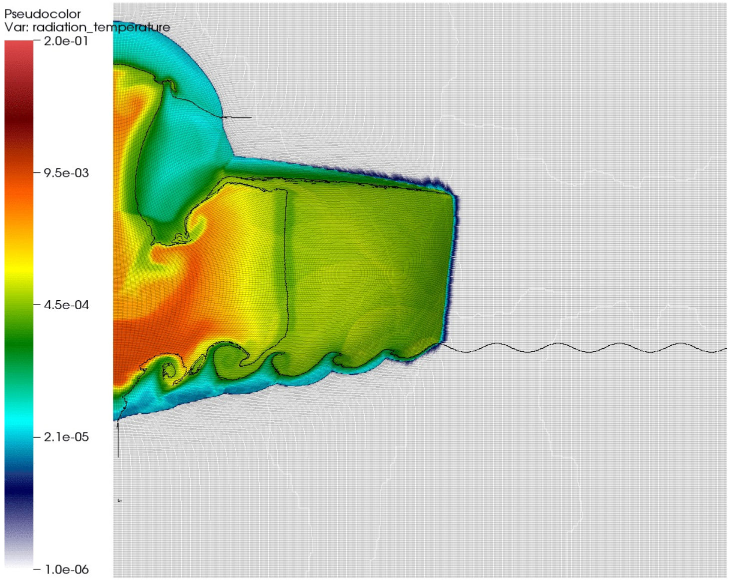




Extension to full ALE radiation hydrodynamics

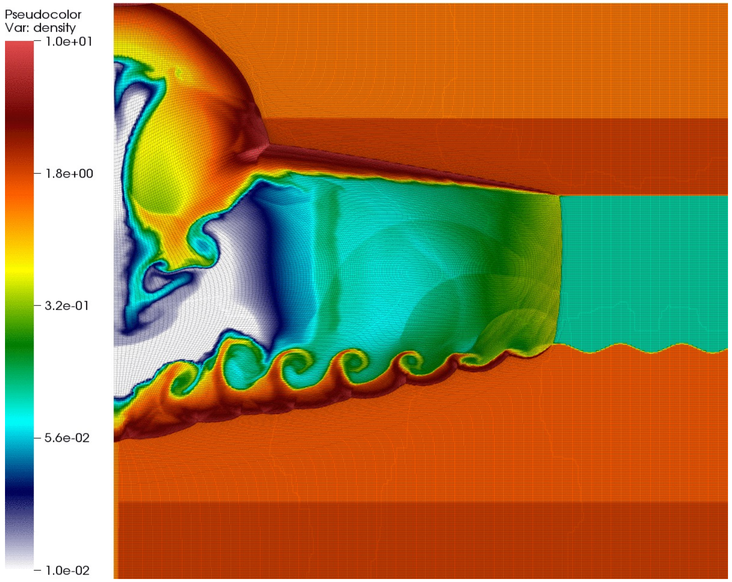
- We simply remap E as a conservative variable (by the FCT advection).
  - There is no need for synchronization with the hydro variables.
  - The radiation flux F is recomputed from the result of the remap.
- Example: radiating Kelvin-Helmholtz instability:
  - 5 materials (ideal gases), Q_2Q_1 discretization, constant opacities.

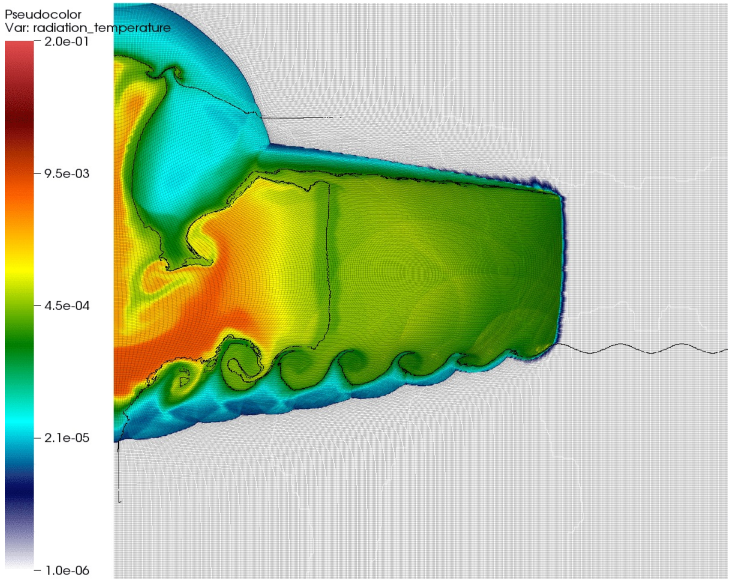




Extension to full ALE radiation hydrodynamics

- We simply remap E as a conservative variable (by the FCT advection).
  - There is no need for synchronization with the hydro variables.
  - The radiation flux F is recomputed from the result of the remap.
- Example: radiating Kelvin-Helmholtz instability:
  - 5 materials (ideal gases), Q_2Q_1 discretization, constant opacities.

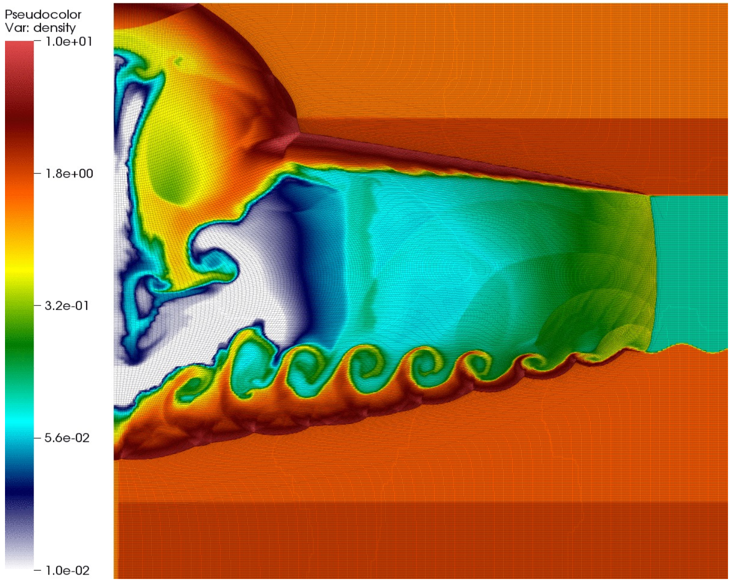


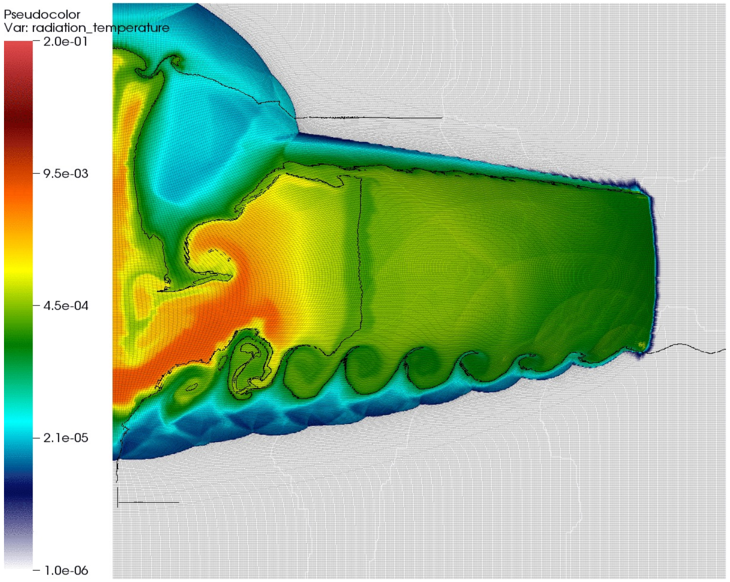


Extension to full ALE radiation hydrodynamics

- We simply remap E as a conservative variable (by the FCT advection).
  - There is no need for synchronization with the hydro variables.
  - The radiation flux F is recomputed from the result of the remap.

- Example: radiating Kelvin-Helmholtz instability:
  - 5 materials (ideal gases), Q_2Q_1 discretization, constant opacities.

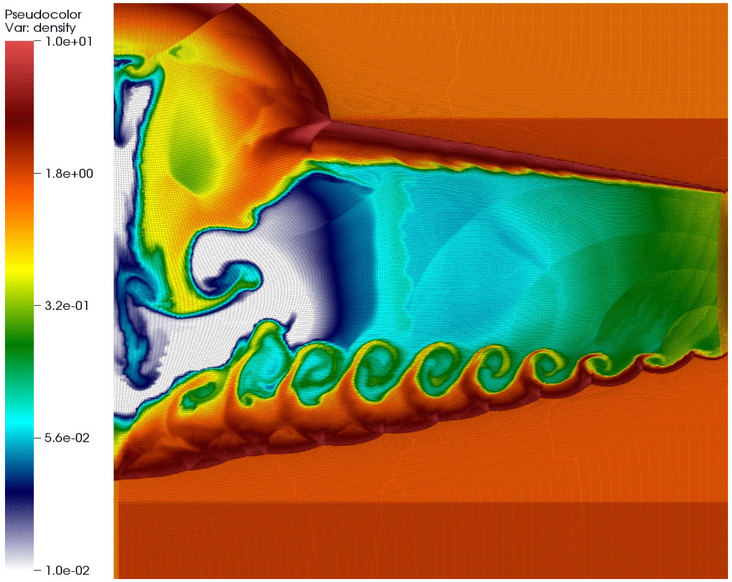


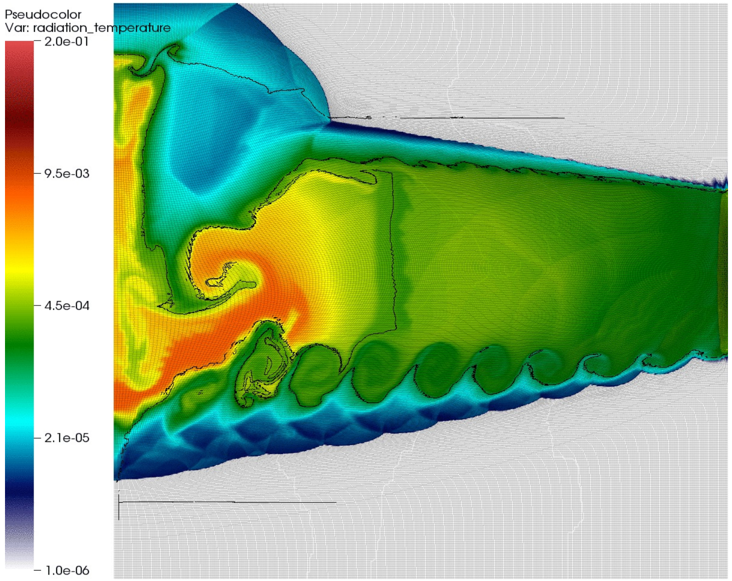


Extension to full ALE radiation hydrodynamics

- We simply remap E as a conservative variable (by the FCT advection).
  - There is no need for synchronization with the hydro variables.
  - The radiation flux F is recomputed from the result of the remap.

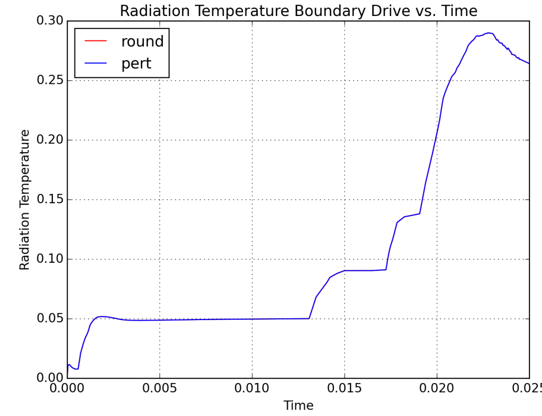
- Example: radiating Kelvin-Helmholtz instability:
  - 5 materials (ideal gases), Q_2Q_1 discretization, constant opacities.

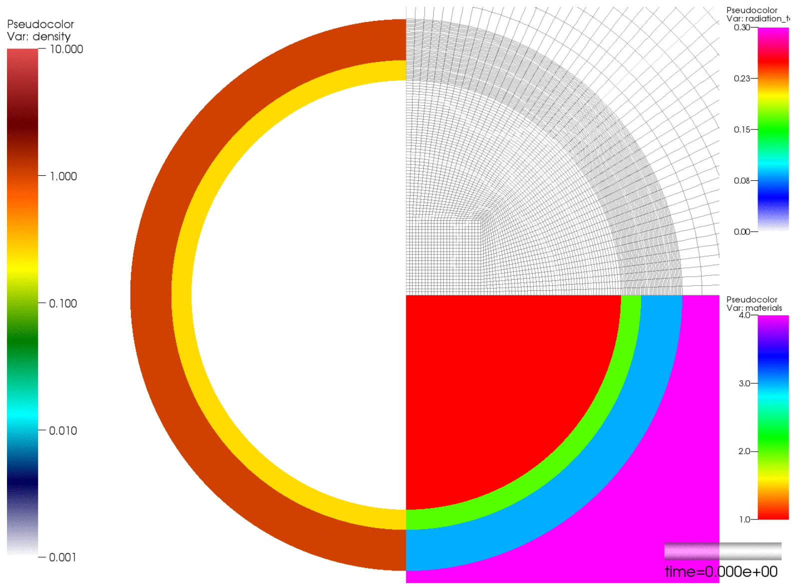


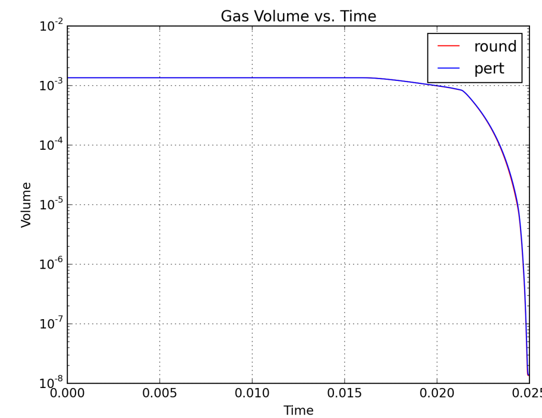


Single group ICF capsule implosion simulation

- 4 materials, tabular EOS, constant material opacities.
  - Originally proposed by R. Tipton.
- Implosion is achieved by a 4-stage temperature drive.
  - The four shock waves collide to achieve the final implosion.
- Results in ≈40 times reduction in the DT-gas radius.

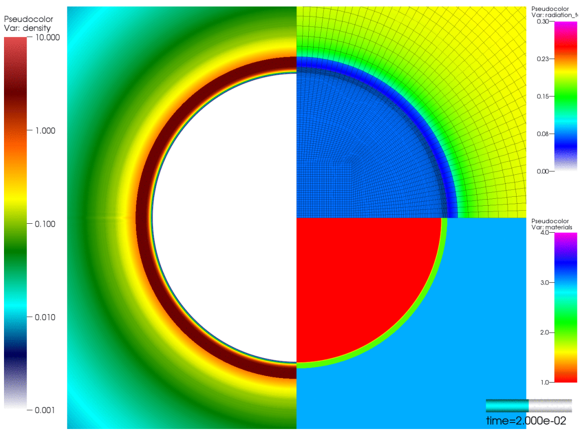


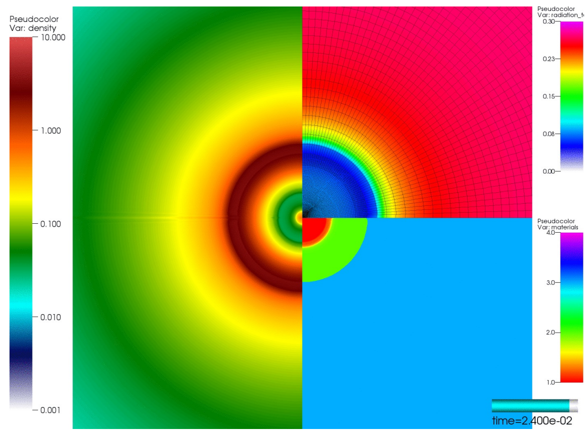


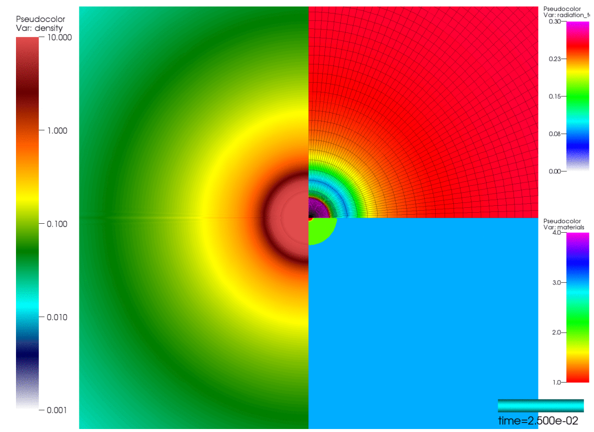


Single group ICF capsule implosion simulation

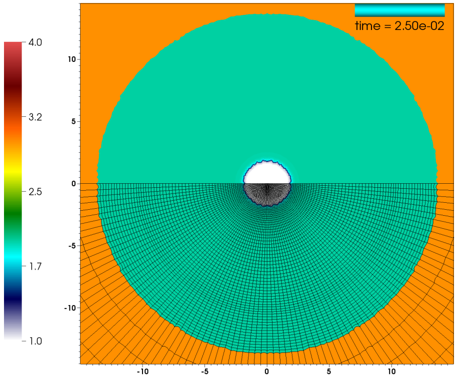
- Density, radiation temperature, material positions at times 2 / 2.4 / 2.5.

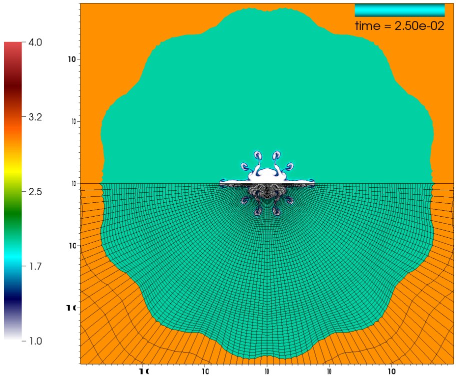






- Final shape of the gas for round / perturbed initial material interfaces.





Summary

- We utilize the $H(div)$ diffusion flux formulation to combine the H^1, L_2 and $H(div)$ high-order finite element spaces.
- We propose two methods for solving the resulting nonlinear system:
  - #1: Elimination of the energy unknowns, $H(div)$ linear solve and back-substitution.
  - #2: block Gauss-Seidel iteration (appropriate for multigroup).
- IMEX time discretization combines explicit hydro and implicit radiation diffusion.
- High-order convergence in space and time for smooth problems.
  - Achieved for thick and thin regimes, structured and unstructured meshes.
- The remap of radiation energy does not complicate the remap phase.
- The method is valid for 2Dxy, 2Drz and 3D unstructured curved meshes, general opacity and material models.

Lawrence Livermore National Laboratory