Multi-material remap algorithms for high-order ALE simulations

7th International Conference on Numerical Methods for Multi-Material Fluid Flow

Veselin Dobrev

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

September 7-11, 2015, Würzburg, Germany

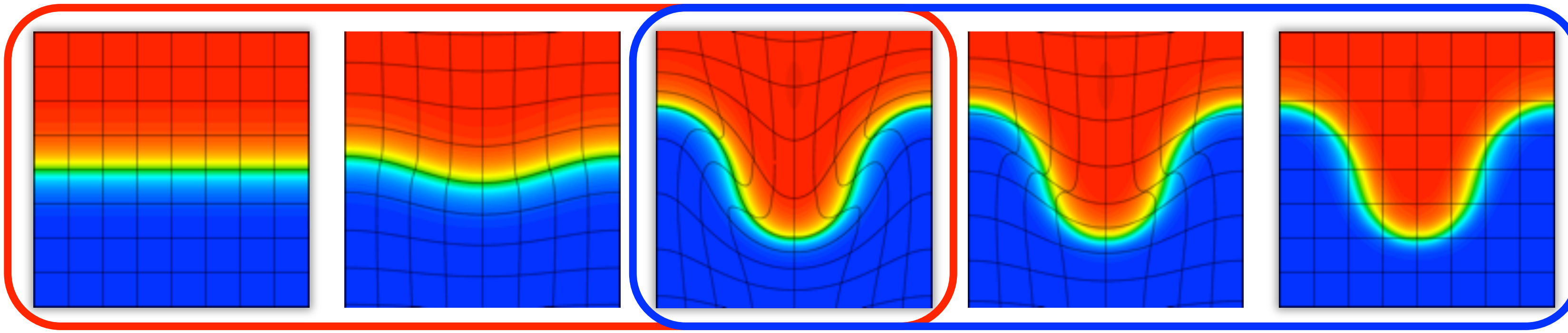
LLNL-PRES-676869

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

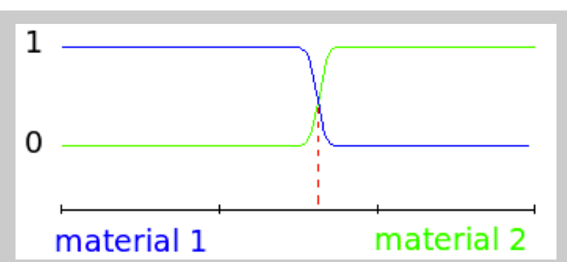
Overview of multi-material arbitrary Lagrangian-Eulerian (ALE) approach

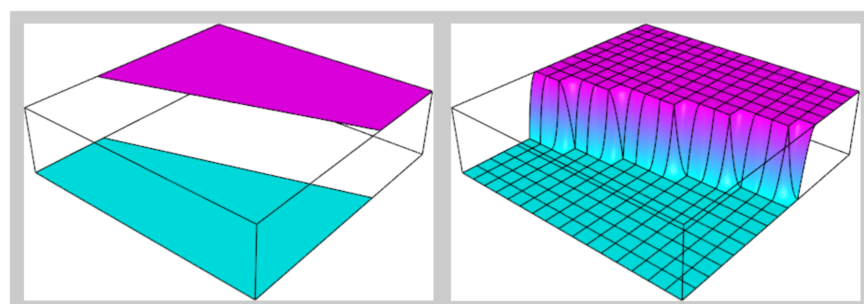
- We develop algorithms for “Lagrange+remap” ALE:



Lagrange phase, physical time t Remap phase, pseudo-time τ

- Materials representation: material indicators





- Discretization: high-order (HO) finite element methods

Overview of Lagrange phase

Solve Euler's equations on a moving mesh with high-order FEM

	Continuous Lagrange	*Semi-discrete* Lagrange
Materials	$\frac{d\eta_k}{dt} = (\beta_k - \eta_k)\nabla \cdot v$	$\mathbf{M}\frac{\mathrm{d}\boldsymbol{\eta}_k}{\mathrm{d}t} = \mathbf{b}_k$
Mass	$\int_V \eta_k \rho_k = \int_{V^0} \eta_k^0 \rho_k^0$	$\eta_k \rho_k \lvert\mathbf{J}\rvert = \eta_k^0 \rho_k^0 \lvert\mathbf{J}^0\rvert$
Energy	$\eta_k \rho_k \frac{de_k}{dt} = \eta_k \sigma_k : \nabla v$	$\mathbf{M_e}\frac{\mathrm{d}\mathbf{e}_k}{\mathrm{d}t} = \mathbf{F}_k^T \cdot \mathbf{v}$
Momentum	$\rho\frac{dv}{dt} = \nabla \cdot \sigma$	$\mathbf{M_v}\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\mathbf{F} \cdot \mathbf{1}$
Position	$\frac{dx}{dt} = v$	$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}$

Physical time evolution

Based on physical motion

Galerkin discretization

Explicit HO time integration

Overview of remap in multi-material ALE

- Fields to remap
  - Material indicators: η_k
  - Densities: ρ_k
  - Specific internal energies: e_k
  - Single velocity: $\vec{v}$
  - Primary vs. conservative variables: $(\eta_k, \eta_k \rho_k, \eta_k \rho_k e_k, \vec{v})$

$$\sum_k \eta_k \equiv 1 \qquad 0 \leq \eta_k \leq 1$$

k – material index

- Requirements
  - Conservation of material *volume, mass, internal energy*; *momentum*:

$$\frac{d}{d\tau} \int \eta_k = 0 \qquad \frac{d}{d\tau} \int \eta_k \rho_k = 0 \qquad \frac{d}{d\tau} \int \eta_k \rho_k e_k = 0 \qquad \frac{d}{d\tau} \int \rho \vec{v} = \vec{0}$$

  - Monotonicity, compatibility:

$$\eta_{k,i}^{\min} \leq \eta_{k,i} \leq \eta_{k,i}^{\max} \qquad \rho_{k,i}^{\min} \leq \frac{(\eta\rho)_{k,i}}{\eta_{k,i}} \leq \rho_{k,i}^{\max} \qquad e_{k,i}^{\min} \leq \frac{(\eta\rho e)_{k,i}}{(\eta\rho)_{k,i}} \leq e_{k,i}^{\max}$$

References

- J. Boris and D. Book, 1973, "*Flux corrected transport. I. SHASTA, A Fluid Transport Algorithm That Works*".
- S. Zalesak, 1979, "*Fully Multidimensional Flux-Corrected Transport Algorithm for Fluids*".
- C. Schar and P. Smolarkiewicz, 1996, "*A Synchronous and Iterative Flux-Correction Formalism for Coupled Transport Equations*".
- D. Kuzmin and S. Turek, 2004, "*High-resolution FEM-TVD schemes based on a fully multidimensional flux limiter*".
- P. Vachal and R. Liska, 2005, "*Sequential Flux-Corrected Remapping for ALE Methods*".
- R. Liska, M. Shashkov, P. Vachal, and B. Wendroff, 2010, "*Optimization-based synchronized flux-corrected conservative interpolation (remapping) of mass and momentum for arbitrary Lagrangian–Eulerian methods*".
- A. Ortega and G. Scovazzi, 2011, "*A geometrically-conservative, synchronized, flux-corrected remap for arbitrary Lagrangian–Eulerian computations with nodal finite elements*".

Remap equations and discretization

Advection-based discontinuous Galerkin (DG)

	Continuous Remap	*Semi-discrete* Remap	
Materials	$\frac{d\eta_k}{d\tau} = u \cdot \nabla \eta_k$	$\mathbf{M}\frac{\mathrm{d}\boldsymbol{\eta}_k}{\mathrm{d}\tau} = \mathbf{K}\boldsymbol{\eta}_k$	
Mass	$\frac{d(\eta_k \rho_k)}{d\tau} = u \cdot \nabla (\eta_k \rho_k)$	$\mathbf{M}\frac{\mathrm{d}(\boldsymbol{\eta}\boldsymbol{\rho})_k}{\mathrm{d}\tau} = \mathbf{K}(\boldsymbol{\eta}\boldsymbol{\rho})_k$	*DG advection of* η_k, ρ_k, e_k
Energy	$\frac{d(\eta_k \rho_k e_k)}{d\tau} = u \cdot \nabla (\eta_k \rho_k e_k)$	$\mathbf{M}\frac{\mathrm{d}(\boldsymbol{\eta}\boldsymbol{\rho}\boldsymbol{e})_k}{\mathrm{d}\tau} = \mathbf{K}(\boldsymbol{\eta}\boldsymbol{\rho}\boldsymbol{e})_k$	
Momentum	$\frac{d(\rho v)}{d\tau} = u \cdot \nabla (\rho v)$	$\mathbf{M}_\mathbf{v}\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}\tau} = \mathbf{K}_\mathbf{v}\mathbf{v}$	*Continuous FE advection of* $\vec{v}$
Position	$\frac{dx}{d\tau} = u$	$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\tau} = \mathbf{u}$	

Zonal DG mass matrix

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

DG advection matrix

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

Global velocity mass matrix

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

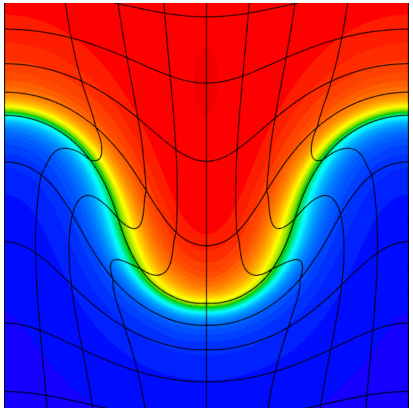
Velocity advection matrix

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

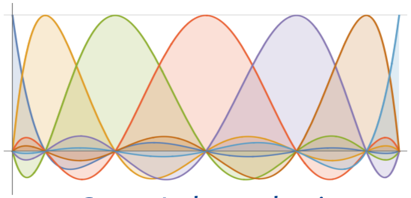
Discretization method

Properties

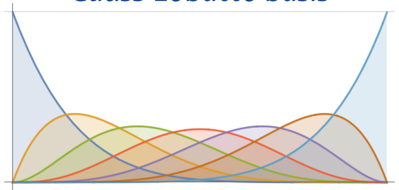
- High-order approximation.
- Conservative on semi-discrete level.
- Preserve constant, linear, and high-order polynomials under suitable conditions.
- Discretization in pseudo-time: high-order RK methods (e.g. SSP).
- Generally not monotone – fix with algebraic FCT
- We use positive (Bernstein) DG basis: important for our algebraic approach.



Q3 remap on Q4 mesh



Gauss-Lobatto basis



Bernstein basis

R. Anderson, V. Dobrev, Tz. Kolev and R. Rieben, ***"Monotonicity in high-order curvilinear finite element arbitrary Lagrangian–Eulerian remap"*** 2014, IJNMF

Algebraic FCT algorithm: low-order method

Discrete upwinding and mass lumping

- A low-order *monotone* method is constructed by defining:

$$\mathbf{M}^* = \mathbf{M}^L = \mathbf{M} + \mathbf{L} \qquad \mathbf{K}^* = \mathbf{K} + \mathbf{D}$$

$$\mathbf{L}_{ij} = \begin{cases} -\mathbf{M}_{ij} & i \neq j \\ \sum_{k\neq i} \mathbf{M}_{ik} & i = j \end{cases} \qquad \mathbf{D}_{ij} = \begin{cases} \max(0, -\mathbf{K}_{ij}, -\mathbf{K}_{ji}) & i \neq j \\ -\sum_{k\neq i} \mathbf{D}_{ik} & i = j \end{cases}$$

- Then the low-order method has the form:

$$\mathbf{M}^* \frac{\mathrm{d}\boldsymbol{\eta}}{\mathrm{d}\tau} = \mathbf{K}^* \boldsymbol{\eta}$$

- For the DG spaces using positive basis, both $\mathbf{L}$ and $\mathbf{D}$ are block-diagonal, i.e. element-wise.

- This low-order method is *compatible*!

Algebraic FCT algorithm

Flux limiting

Consider a forward Euler discretization for both high-order and low-order solutions:

$$\mathbf{M}\Delta\boldsymbol{\eta}^H = \Delta\tau\mathbf{K}\boldsymbol{\eta}$$

$$\mathbf{M}^*\Delta\boldsymbol{\eta}^L = \Delta\tau\mathbf{K}^*\boldsymbol{\eta}$$

The high-order solution can be written as:

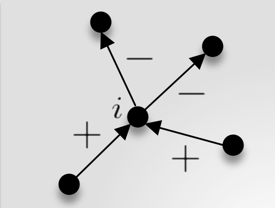
$$\mathbf{M}^*\Delta\boldsymbol{\eta}^H = \mathbf{M}^*\Delta\boldsymbol{\eta}^L + (\mathbf{M}^* - \mathbf{M})\Delta\boldsymbol{\eta}^H - \Delta\tau\mathbf{D}\boldsymbol{\eta}$$

We have anti-symmetric high-order flux correction:

$$\mathbf{f}_{ij} = \mathbf{M}_{ij}(\Delta\boldsymbol{\eta}_i^H - \Delta\boldsymbol{\eta}_j^H) + \Delta\tau\mathbf{D}_{ij}(\boldsymbol{\eta}_i - \boldsymbol{\eta}_j)$$

We can apply a symmetric (conservative) scaling factor

$$\mathbf{M}^*_{ii}\Delta\boldsymbol{\eta}_i = \mathbf{M}^*_{ii}\Delta\boldsymbol{\eta}_i^L + \sum_{j\neq i}\alpha_{ij}\mathbf{f}_{ij}$$



per-DOF flux network

Scaling based on worst case scenario of all positive/negative fluxes contributing together

$$\alpha_{ij} = \begin{cases} \min\left(\alpha_i^+, \alpha_j^-\right) & \mathbf{f}_{ij} > 0 \\ \min\left(\alpha_i^-, \alpha_j^+\right) & \mathbf{f}_{ij} < 0. \end{cases}$$

$$\alpha_i^\pm = \min\left(1, \frac{\Delta\boldsymbol{\eta}^{A\pm,\max}}{\Delta\boldsymbol{\eta}^{A\pm}}\right)$$

$$\Delta\boldsymbol{\eta}_i^{A+,\max} = \boldsymbol{\eta}_i^{\max} - \boldsymbol{\eta}_i^L$$

$$\mathbf{M}^*_{ii}\Delta\boldsymbol{\eta}_i^{A+} = \sum_{\mathbf{f}_{ij}>0}\mathbf{f}_{ij}$$

Iterated FCT: $$\mathbf{M}^*_{ii}\Delta\boldsymbol{\eta}_i^H = \mathbf{M}^*_{ii}\Delta\boldsymbol{\eta}_i + \sum_{j\neq i}(1-\alpha_{ij})\mathbf{f}_{ij}$$

Compatible FCT algorithm

Primary field compatibility constraints, imposed at DOFs

$$\boldsymbol{\rho}_i^{\min} \leq \frac{(\boldsymbol{\eta\rho})_i}{\boldsymbol{\eta}_i} \leq \boldsymbol{\rho}_i^{\max}$$

Remap phase

Satisfies the bounds!

Average zonal density

Compatible low-order field

$$(\boldsymbol{\eta\rho})_{z,i}^{LC} = \boldsymbol{\eta}_{z,i}\overline{\boldsymbol{\rho}}_z \qquad \overline{\boldsymbol{\rho}}_z = \frac{\boldsymbol{m}_z \cdot (\boldsymbol{\eta\rho})_z^L}{\boldsymbol{m}_z \cdot \boldsymbol{\eta}_z} \qquad \boldsymbol{m} = \mathbf{M}^* \mathbf{1}$$

Compatible low-order fluxes

$$\boldsymbol{f}_{ij}^C = \boldsymbol{f}_{ij} + (\boldsymbol{x}_j - \boldsymbol{x}_i) \qquad \boldsymbol{x} = \frac{1}{n}\mathbf{M}^* \left((\boldsymbol{\eta\rho})^{LC} - (\boldsymbol{\eta\rho})^L\right)$$

Apply FCT with compatible low-order field and fluxes

$$\mathbf{M}^*(\boldsymbol{\eta\rho}) = \mathbf{M}^*(\boldsymbol{\eta\rho})^{LC} + \sum_j \alpha_{ij}\boldsymbol{f}_{ij}^C$$

Limiting factors based on the density bounds

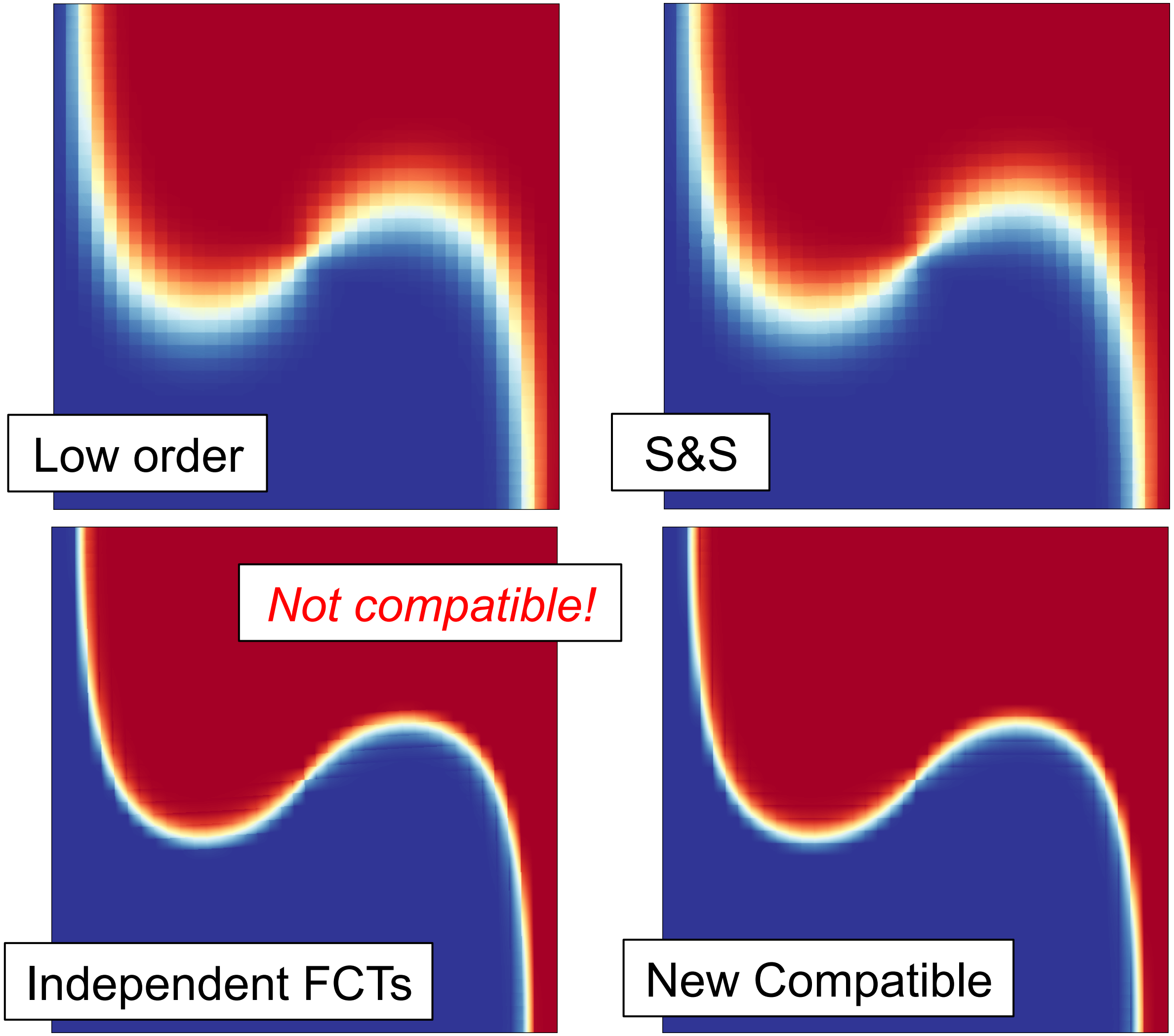
- Similar treatment for the energy $(\boldsymbol{\eta\rho}\mathrm{e})$ using $(\boldsymbol{\eta\rho})$
- Similar treatment for post-Lagrange $(\boldsymbol{\eta}, \boldsymbol{\rho}, \boldsymbol{e}) \rightarrow (\boldsymbol{\eta}, \boldsymbol{\eta\rho}, \boldsymbol{\eta\rho e})$
- Alternative: the compatible method of Schar and Smolarkiewicz (S&S)

Numerical test

Material indicator in 2D Taylor-Green vortex problem

- Q2-Q1 method
- 40x40 mesh
- Artificial vertical material interface at t=0
- Final time t=0.75
- All cases use the compatible post-Lagrange transition

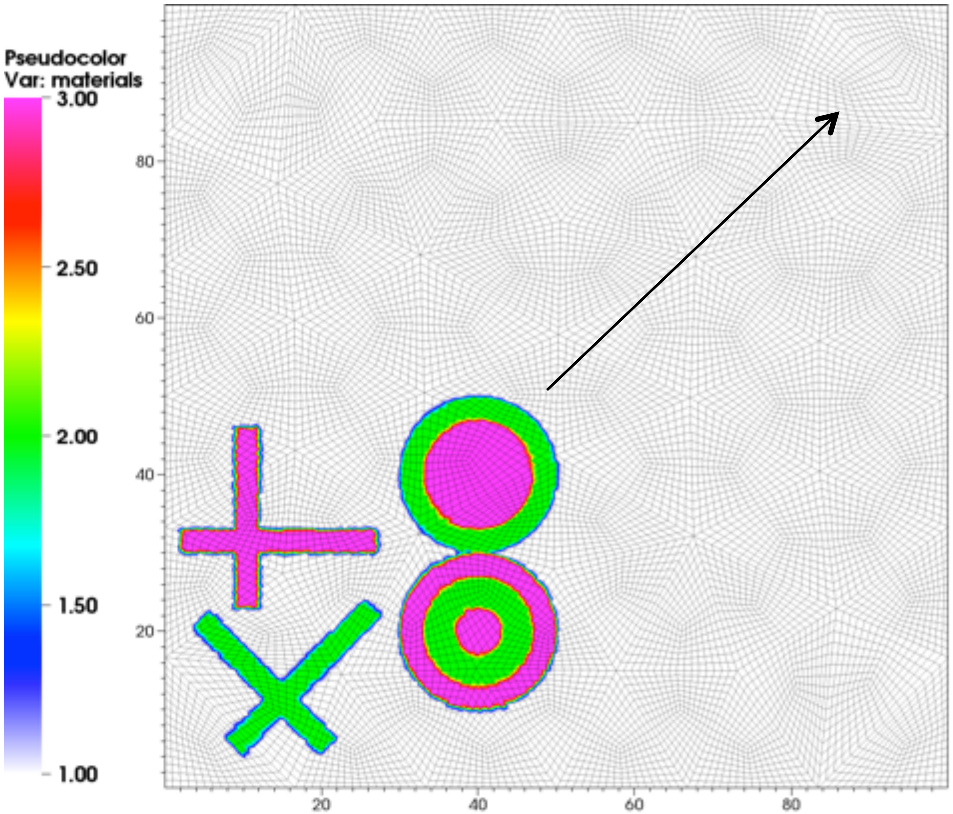
All tests were performed with the BLAST code



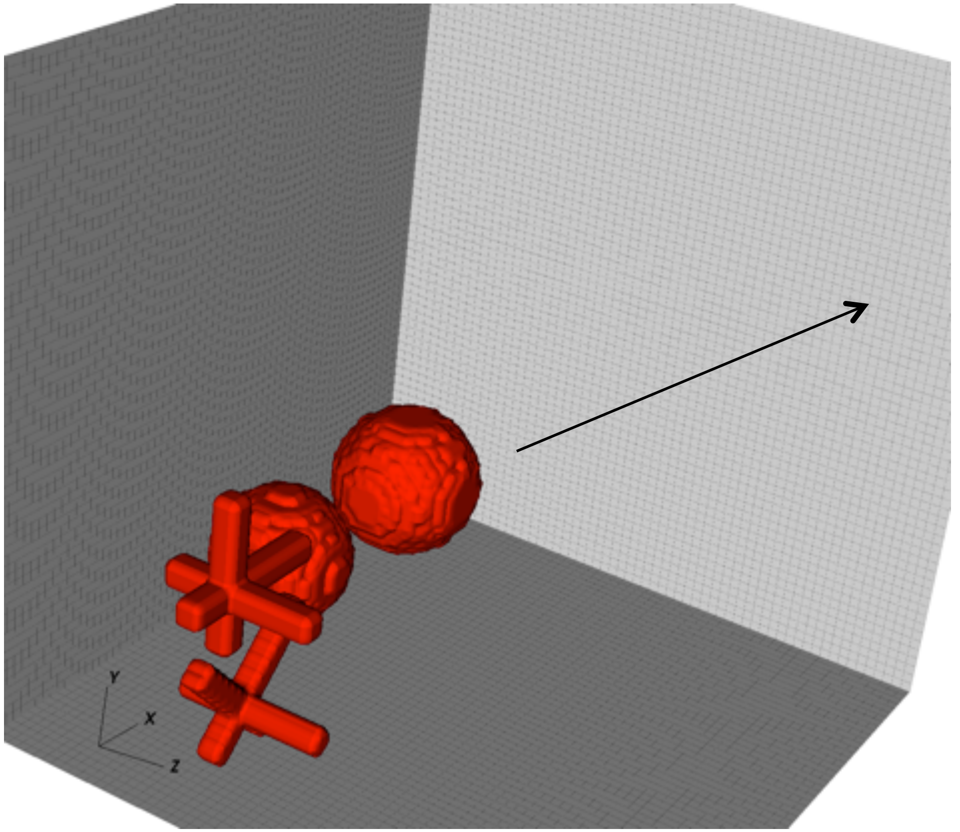
Numerical test

Material indicators advection

Initial material indicators



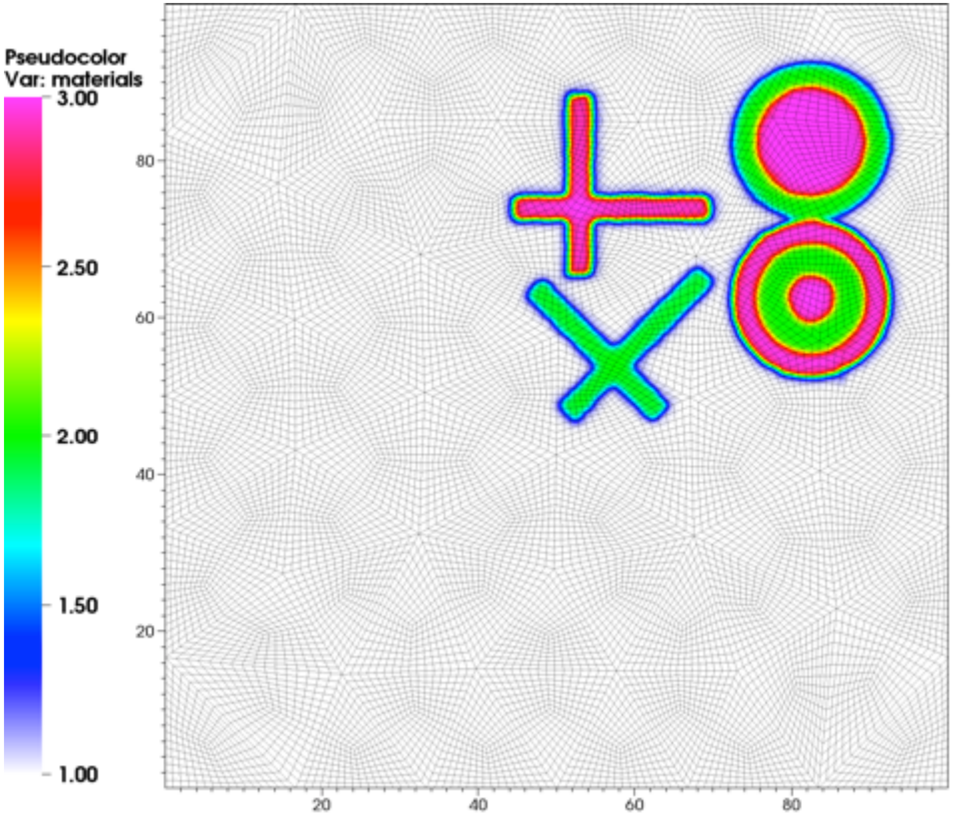
Q3 indicators, unstructured 2D mesh



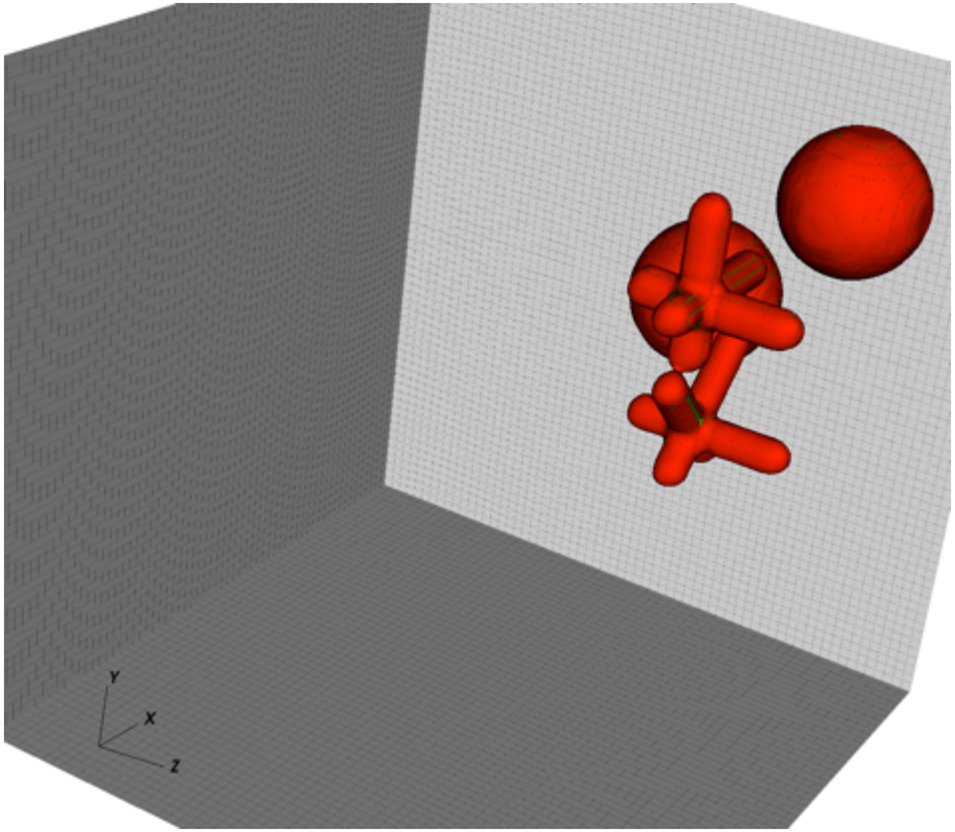
Q2 indicators, 64^3 mesh

Numerical test
Material indicators advection

Final material indicators



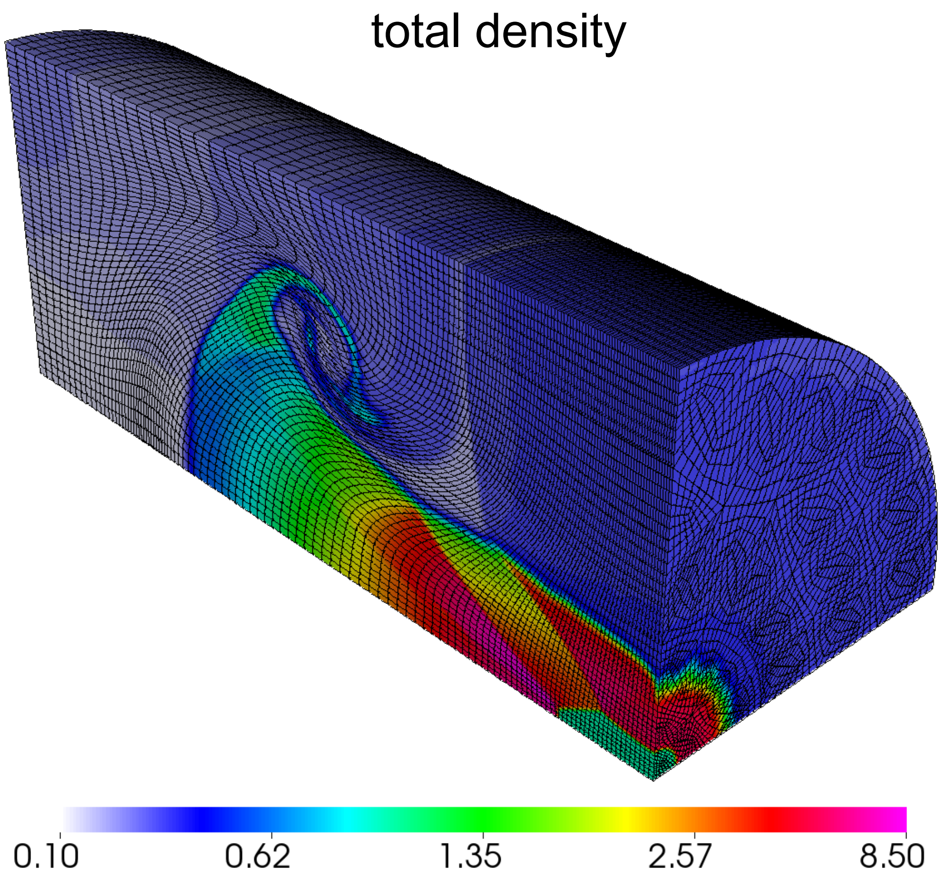
Q3 indicators, unstructured 2D mesh

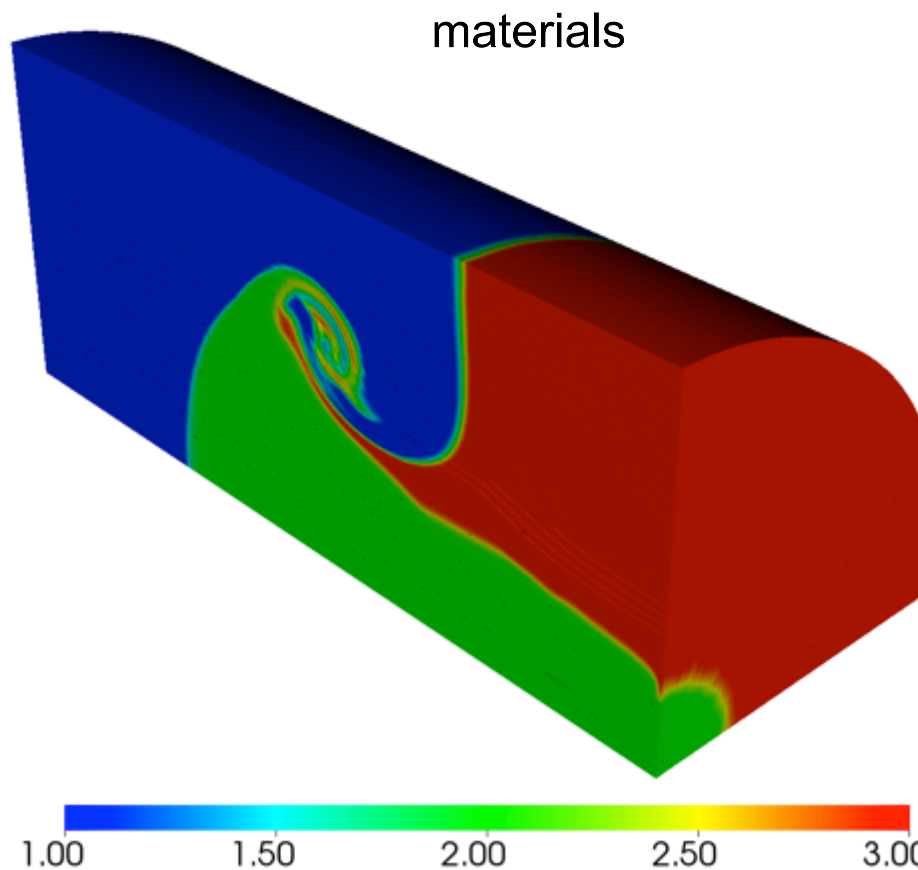


Q2 indicators, 64^3 mesh

Numerical test

3D unstructured multi-material triple point problem



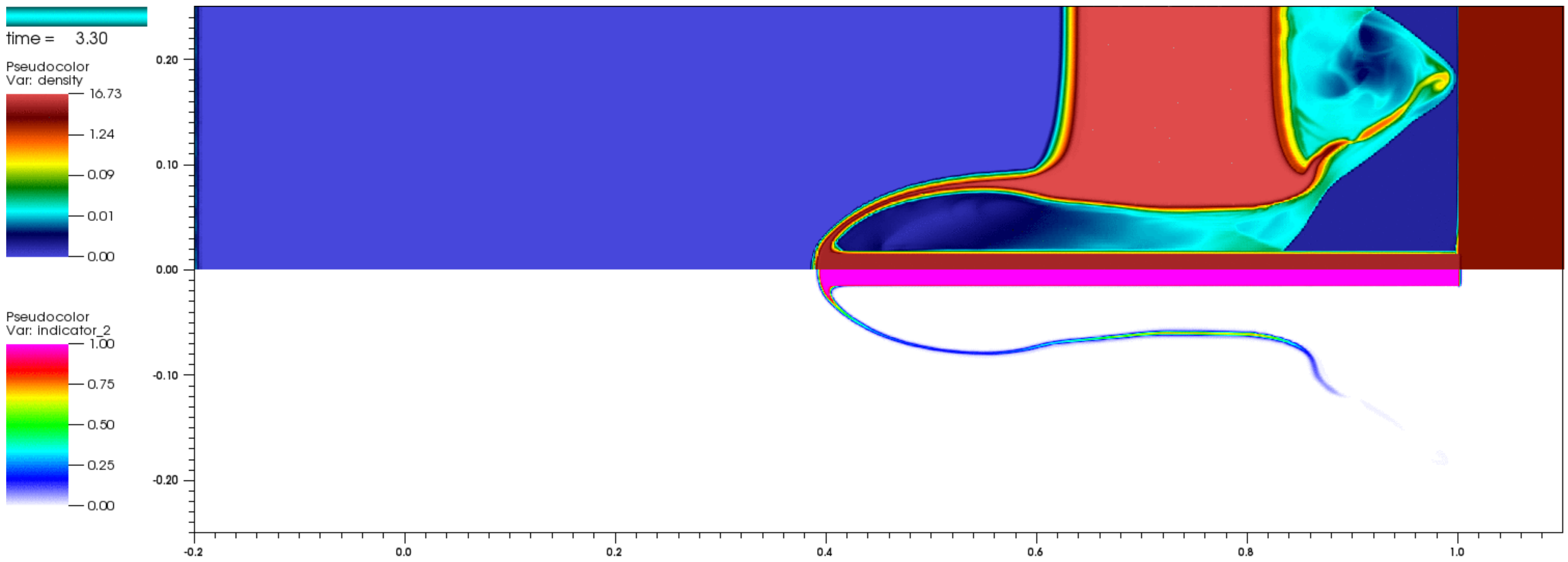


- Q2-Q1 + Q2 indicators, RK2 Lag, RK2 remap, hyper-viscosity limiter, ale_period 40 + neo-Hookean non-linear relaxation
- 256 processors, 6,340 cycles, 2.71 seconds/cycle

Numerical test

Axisymmetric flyer-plate rod impact

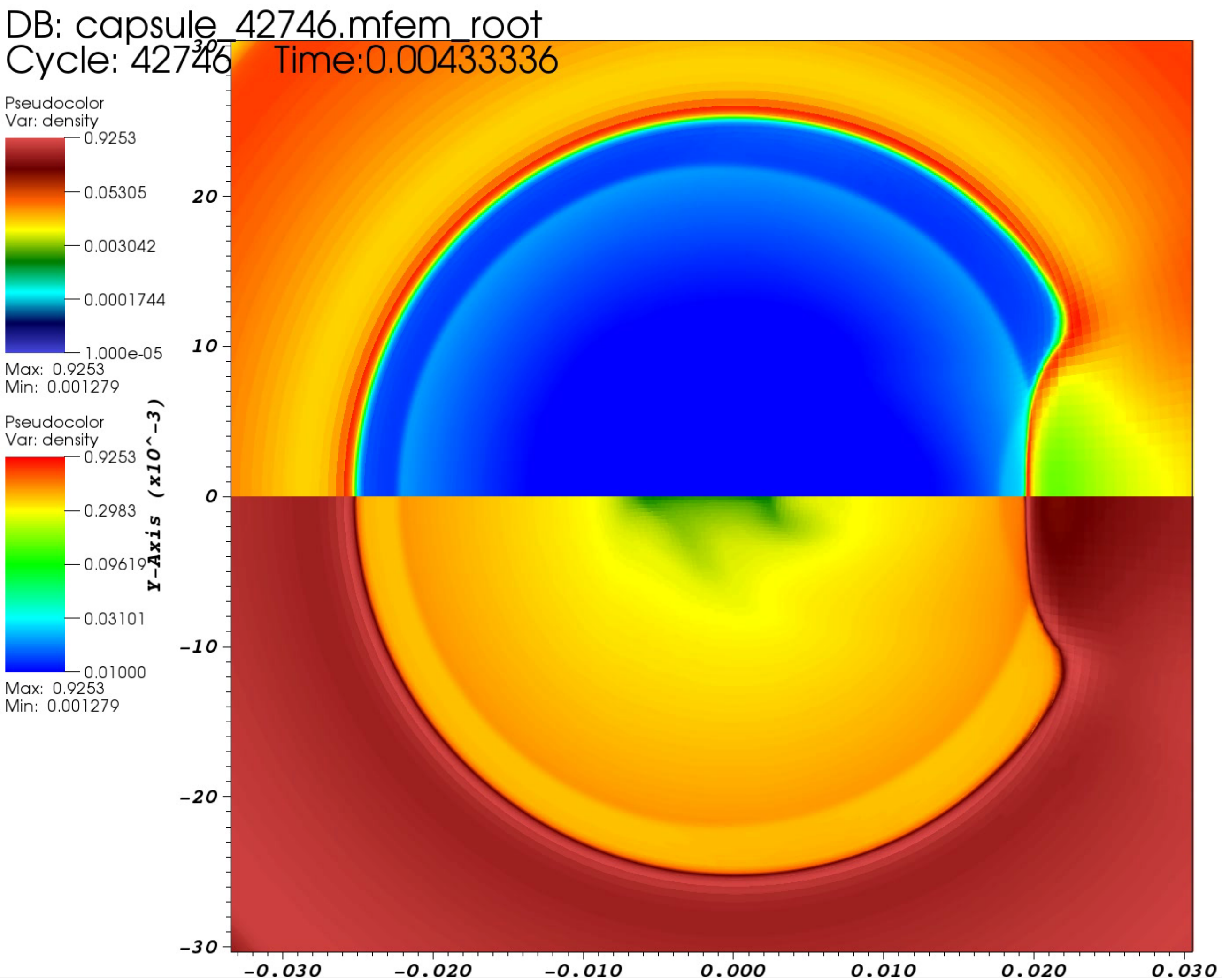
D. Haylett et. al. flyer-plate rod impact experiment



Multi-material Q2 Eulerian simulation

NIC capsule with with jet through origin

Hydrodynamics-only (thanks to A. Kaptanoglu, S. Langer)



Element based FCT

Algorithm summary (with D. Kuzmin and M. Quezada de Luna)

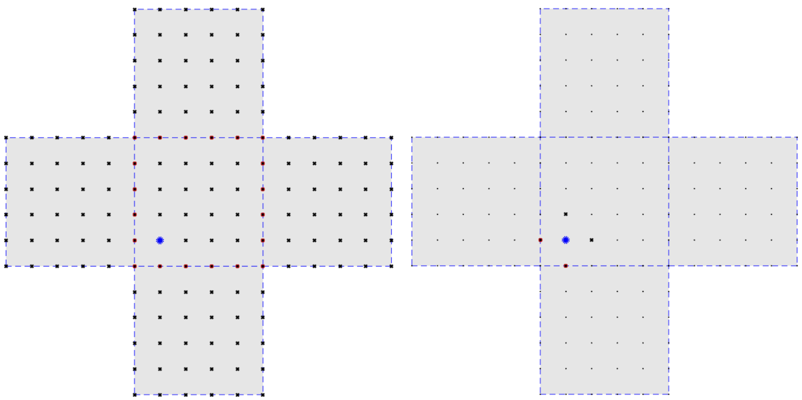
High-order "point" fluxes:

$$\mathbf{M}^*_{ii}(\boldsymbol{\eta}^H_i - \boldsymbol{\eta}^L_i) = \mathbf{f}^H_i$$

$$\sum_{i \in K} \mathbf{f}^H_i = 0 \leftarrow$$

The fluxes are conservative on each element

Use smaller neighborhood:



Used to define $\boldsymbol{\eta}^{\min}, \boldsymbol{\eta}^{\max}$

Clipped HO solution/fluxes:

$$\boldsymbol{\eta}^*_i = \min\left(\boldsymbol{\eta}^{\max}_i, \max\left(\boldsymbol{\eta}^{\min}_i, \boldsymbol{\eta}^H_i\right)\right)$$
$$\mathbf{f}^*_i = \mathbf{M}^*_{ii}(\boldsymbol{\eta}^*_i - \boldsymbol{\eta}^L_i)$$

Conservation is lost!

Recover conservation locally:

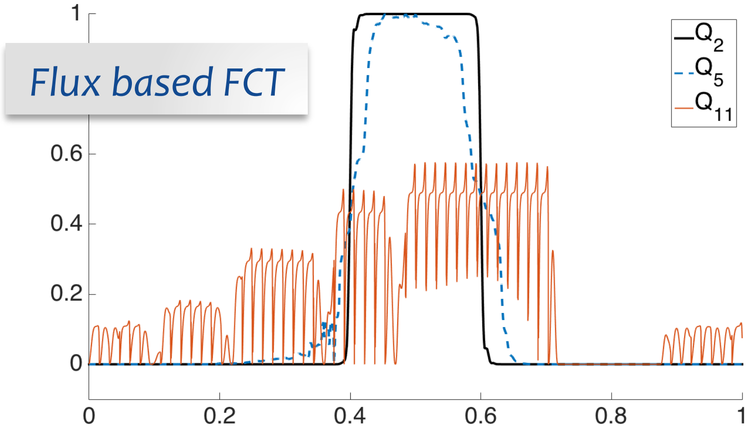
$$\mathbf{M}^*_{ii}(\boldsymbol{\eta}_i - \boldsymbol{\eta}^L_i) = \alpha_i \mathbf{f}^*_i$$
$$\mathbf{M}^*_{ii}(\boldsymbol{\eta}_i - \boldsymbol{\eta}^L_i) = \mathbf{f}^*_i - \lambda_K \mathbf{z}_i$$

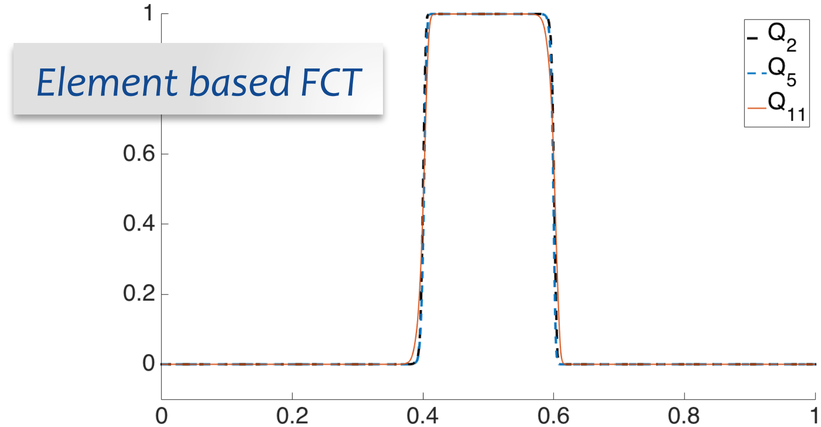
$$\mathbf{z}_i = \mathbf{w}_i + \mathbf{f}^*_i / \lambda_K \min(0, 1 - \lambda_K \mathbf{w}_i / \mathbf{f}^*_i)$$

- choose same α_i or
- solve an equation for λ_K

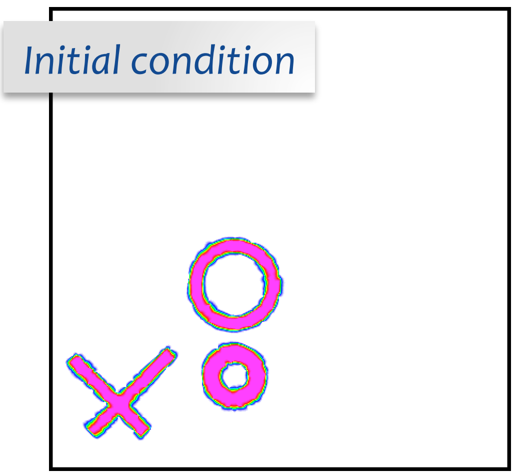
Element based FCT

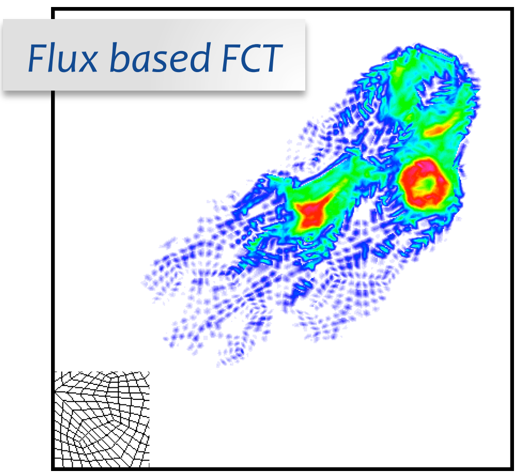
Results

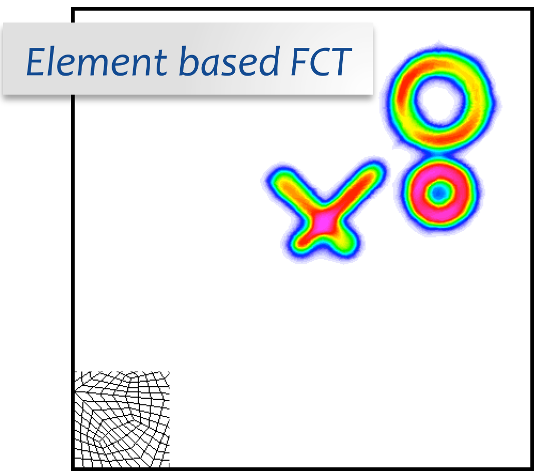




Q5:







Summary

- We have developed multi-material remap algorithm for high-order meshes and fields that:
  - Based on material indicator functions
  - Does not require interface reconstruction
  - Interpolates (remaps) the conserved variables
  - Uses high-order advection-based DG discretization
  - Utilizes compatible algebraic FCT monotonicity algorithm
- Future work:
  - Multi-material element based FCT remap
  - Improve monotonicity algorithm for higher orders
  - Exact conservation on fully discrete level
- Papers and additional information:
  - BLAST project, http://www.llnl.gov/casc/blast
  - FEM software, http://mfem.org
- More about BLAST in *T. Kolev's talk* (closure models) and *R. Rieben's poster* (performance optimizations, applications)