A Direct ALE Approach for MultiMaterial Flows on Unstructured Grids

Jacob Waltz

Los Alamos National Laboratory

Collaborators: Tom Canfield, Marc Charest, Nathaniel Morgan, and John Wohlbier

LA-UR-15-26843

A direct ALE method for multi-material flows on unstructured grids is under development

- Based on the generalization of a single-material Godunov scheme to multiple materials
- Key features
  - Direct solution of the multi-material ALE hydro equations
  - Approximate Riemann solvers in moving reference frame
  - Mesh velocity based on local fluid velocity with smoothing
  - Algebraic treatment of volume fraction equation
- Preliminary results on initial test problems have been obtained
  - Multiple interface methods under investigation
  - Further testing/validation is in progress

The ALE algorithm solves the flux-conservative Euler equations written for a moving reference frame

- The velocity of the reference frame is denoted by w_i with Eulerian and Lagrangian treated as limits

$$\frac{1}{V}\left[\frac{\partial(V\rho)}{\partial t}\right]_w + \frac{\partial}{\partial x_i}\left[\rho\left(u_i - w_i\right)\right] = 0$$

$$\frac{1}{V}\left[\frac{\partial(V\rho u_i)}{\partial t}\right]_w + \frac{\partial}{\partial x_j}\left[\rho u_i\left(u_j - w_j\right) + \delta_{ij} p\right] = 0$$

$$\frac{1}{V}\left[\frac{\partial(V\rho E)}{\partial t}\right]_w + \frac{\partial}{\partial x_i}\left[\rho E\left(u_i - w_i\right) + u_i p\right] = 0$$

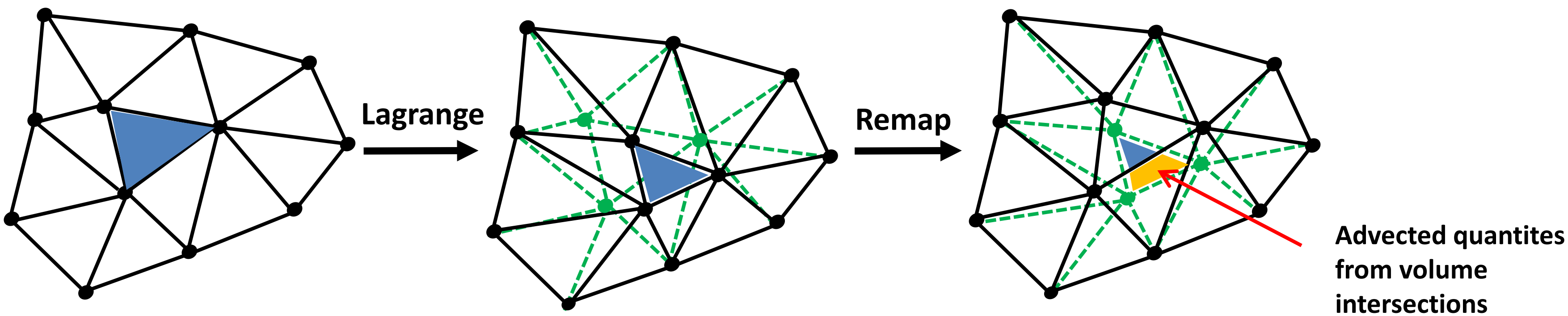
Lagrangian limit: $w_i = u_i$
Eulerian limit: $w_i = 0$

- Or in a more compact vector notation

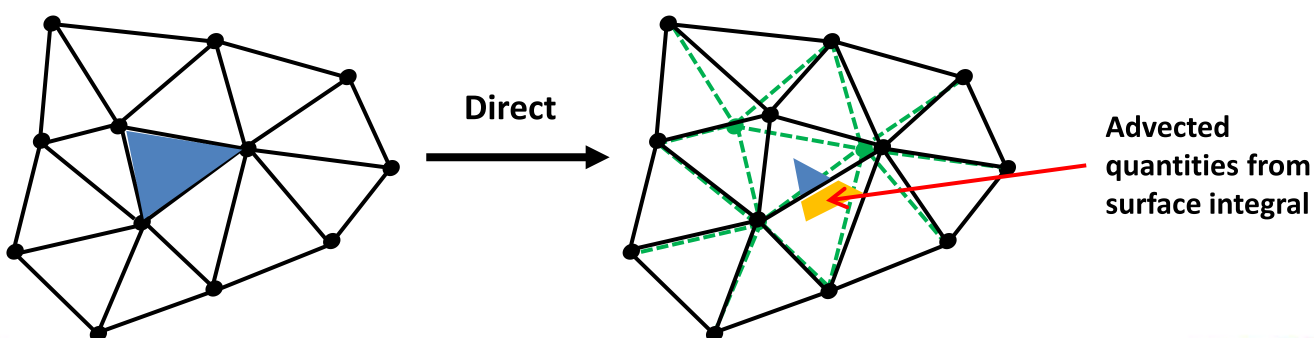
$$\frac{1}{V}\frac{\partial\left(V\overline{U}\right)}{\partial t} + \frac{\partial \overline{F}_j}{\partial x_j} = 0 \qquad \overline{U} = \begin{pmatrix} \rho \\ \rho u_i \\ \rho E \end{pmatrix} \qquad \overline{F}_j = \begin{bmatrix} \rho\left(u - w\right)_j \\ \rho u_i\left(u - w\right)_j + \delta_{ij} p \\ \rho E\left(u - w\right)_j + u_j p \end{bmatrix}$$

The hydro equations are solved directly in the moving reference frame with no Lagrange step

- Lagrange-plus-remap: Mesh moves with fluid in Lagrange step, then relative to the fluid in remap step



- Direct ALE: Mesh moves independently of fluid at its own velocity



$$\int_{\Gamma} \begin{bmatrix} \rho(u_j - w_j) \\ \rho u_i(u_j - w_j) \\ \rho E(u_j - w_j) \end{bmatrix} d\Gamma_j$$

The multi-material extension adds equations for the volume fraction α_k

- Hydro equations are written for a material *k*
  - Separate thermodynamic state for each material in a control volume
  - Single fluid velocity and momentum equation applied as a closure

$$\frac{1}{V}\frac{\partial\left(V\overline{U}\right)}{\partial t}+\frac{\partial \overline{F}_j}{\partial x_j}=\overline{S}$$

$$\overline{U}=\begin{pmatrix}\alpha_k\\ \rho_k\alpha_k\\ \rho_k\alpha_k u_i\\ \rho_k\alpha_k E_k\end{pmatrix}\qquad \overline{F}_j=\begin{bmatrix}\alpha_k\left(u-w\right)_j\\ \rho_k\alpha_k\left(u-w\right)_j\\ \rho_k u_i\left(u-w\right)_j+\delta_{ij}p\\ \rho_k\alpha_k E_k\left(u-w\right)_j+\alpha_k u_j p_k\end{bmatrix}\qquad \overline{S}=\begin{pmatrix}\alpha_k\dfrac{\partial u_i}{\partial x_i}\\ 0\\ 0\\ p_k u_i\dfrac{\partial \alpha_k}{\partial x_i}\end{pmatrix}$$

Advection is computed directly as part of the system of equations instead of from volume intersections

- Eulerian form of volume fraction equation:

$$\frac{\partial \alpha_k}{\partial t} + u_i \frac{\partial \alpha_k}{\partial x_i} = 0$$

- Transform to moving reference frame:

$$\left.\frac{\partial}{\partial t}\right|_w = \frac{\partial}{\partial t} + w_i \frac{\partial}{\partial x_i} \rightarrow \left.\frac{\partial \alpha_k}{\partial t}\right|_w + \left(u_i - w_i\right)\frac{\partial \alpha_k}{\partial x_i} = 0$$

- Rewrite in flux-conservative form (and dropping the *w* subscript):

$$\frac{1}{V}\frac{\partial\left(V\alpha_k\right)}{\partial t} + \frac{\partial}{\partial x_i}\left[\alpha_k\left(u_i - w_i\right)\right] = \alpha_k \frac{\partial u_i}{\partial x_i}$$

UNCLASSIFIED

The ALE equations are discretized with an edge-based Finite Element method for linear tetrahedra

- Semi-discrete weak Galerkin formulation with element-based stencil :

$$\frac{d}{dt}(V\bar{U})^v + \sum_{\Omega_h \in v} \left\{ \sum_{w \in \Omega_h} \int_{\Omega_h} N^v \frac{\partial N^w}{\partial x_j} d\Omega_h \cdot \left(\overline{F_j}\right)^w \right\} = 0$$

sum over elements Ω_h surrounding node *v*

sum over nodes *w* contained in Ω_h

- Algebraically equivalent edge-based stencil:

$$\frac{d}{dt}(V\bar{U})^v + \sum_{vw \in v} \left\{ \left[\frac{1}{2} \sum_{\Omega_h \in vw} \int_{\Omega_h} \left(\frac{\partial N^v}{\partial x_j} N^w - N^v \frac{\partial N^w}{\partial x_j} \right) d\Omega_h \right] \cdot \left[\underbrace{\left(\overline{F_j}\right)^v + \left(\overline{F_j}\right)^w}_{} \right] \right\} = 0$$

sum over edges *vw* surrounding node *v*

sum over elements Ω_h surrounding *vw*

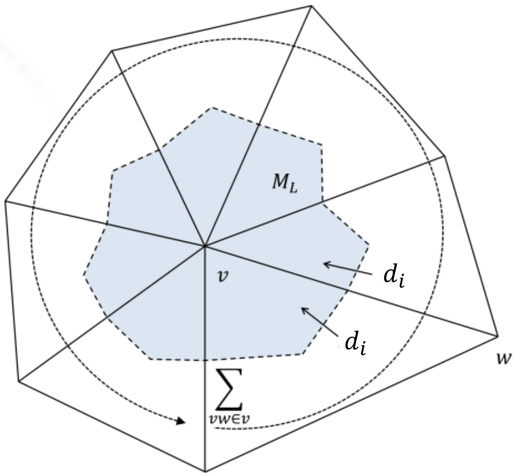
Replaced with flux from Riemann solver

Consistency and conservation are ensured *by construction* for all choices of mesh velocity

- Semi-discrete equation for mesh point *v* is written with a single Riemann flux $\bar{F}_i^{vw}$ on each edge as

$$\frac{d}{dt}(V\bar{U})^v + \sum_{vw\in v} D_i^{vw}\,\bar{F}_i^{vw} = 0$$

$$D_i^{vw} = \frac{1}{2}\sum_{\Omega_h\in vw}\int_{\Omega_h}\left(\frac{\partial N^v}{\partial x_j}N^w - N^v\frac{\partial N^w}{\partial x_j}\right)d\Omega_h = \frac{1}{2}\sum_{\Omega_h\in vw} d_i^{vw,\Omega_h}$$



Edge-based stencil in 2D

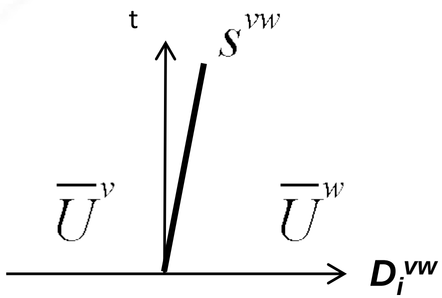
- Consistency and conservation statements:

$$\lim_{\Omega_h\to 0}\left[\frac{d}{dt}(V\bar{U})^v + \sum_{vw\in v} D_i^{vw}\,\bar{F}_i^{vw}\right] = \int_{\Omega}\frac{1}{V}\frac{\partial(V\bar{U})}{\partial t}d\Omega + \int_{\Gamma}\bar{F}_i d\Gamma_i \quad \forall\, w_i$$

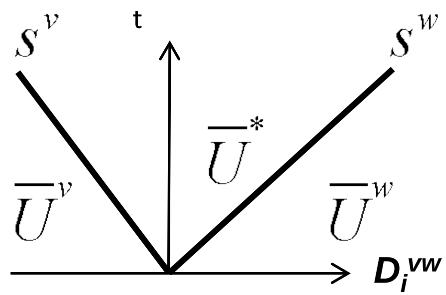
$$D_i^{wv}\bar{F}_i^{vw} = -D_i^{vw}\bar{F}_i^{vw} \qquad \forall\, w_i$$

A directionally unsplit flux on each edge is computed from an approximate Riemann problem along D_i^{vw}

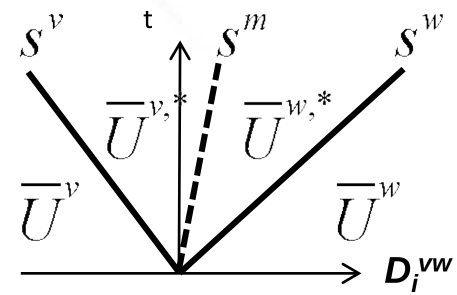
- Rusanov, HLL, and HLLC schemes have been implemented



1D Riemann problem (Rusanov)



1D Riemann problem (HLL)



1D Riemann problem (HLLC)

- Rusanov equations (shown for simplicity):

$$s^{v} = \left| \left(u_i^{v} - w_i^{v}\right) \frac{D_i^{vw}}{\left|D_i^{vw}\right|} \right| + c^{v}; \quad s^{w} = \left| \left(u_i^{w} - w_i^{w}\right) \frac{D_i^{vw}}{\left|D_i^{vw}\right|} \right| + c^{w}; \quad s^{vw} = \max\left(s^{v}, s^{w}\right)$$

$$D_i^{vw} \overline{F}_i^{vw} = D_i^{vw} \left(\overline{F}_i^{v} + \overline{F}_i^{w}\right) + \left|D_i^{vw}\right| s^{vw} \left(\overline{U}^{w} - \overline{U}^{v}\right)$$

A MUSCL reconstruction on primitive variables is used to obtain a second-order upwind method

- Given a field variable f with nodal values f^v and f^w, the reconstruction on edge vw is written as

$$\tilde{f}^v = f^v + \frac{1}{4}\left[(1+k)\phi\left(r^v\right)\delta_1 + (1-k)\phi\left(\frac{1}{r^v}\right)\delta_2\right]$$

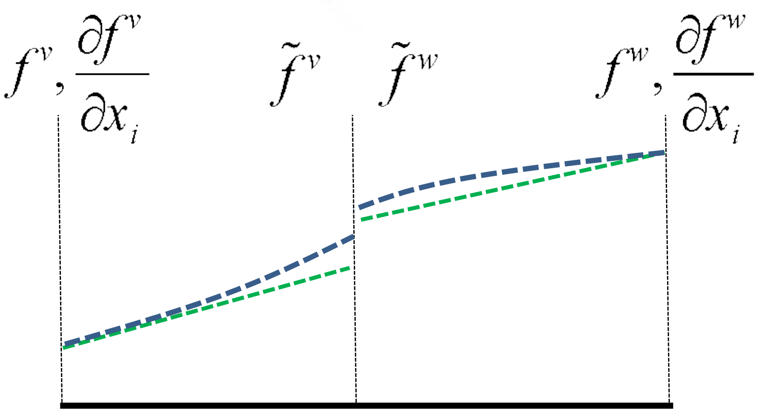
$$\tilde{f}^w = f^w - \frac{1}{4}\left[(1+k)\phi\left(r^w\right)\delta_3 + (1-k)\phi\left(\frac{1}{r^w}\right)\delta_2\right]$$

$$\delta_1 = 2x_i^{vw}\frac{\partial f^v}{\partial x_i} - \delta_2$$

$$\delta_2 = f^w - f^v$$

$$\delta_3 = 2x_i^{vw}\frac{\partial f^w}{\partial x_i} - \delta_2$$

ϕ is any symmetric TVD limiter



Piecewise linear: k = -1
Piecewise parabolic: k = 1/3

UNCLASSIFIED

The semi-discrete ALE equations are integrated in time with an explicit multi-stage scheme

- Difference formula:

$$\left(V\overline{U}\right)^{v,0} = \left(V\overline{U}\right)^{v,n}$$

$$\alpha^k = \frac{1}{1+m-k}$$

$$\left(V\overline{U}\right)^{v,k} = \left(V\overline{U}\right)^{v,0} - \alpha^k \Delta t \left(\sum_{vw \in v} D_i^{vw} \overline{F}_i^{vw}\right)^{k-1}$$

$$\left(V\overline{U}\right)^{v,n+1} = \left(V\overline{U}\right)^{v,m}$$

where *m* is the total number of stages and $1 \le k \le m$

- Same scheme used for mesh motion

- Summary of ALE step
  1. Compute mesh velocity
  2. Compute gradients
  3. On each edge:
     a. Compute MUSCL reconstruction
     b. Compute flux from Riemann solver
  4. Sum flux increments to points
  5. Update $V\overline{U}$ to *n+1*
  6. Update geometry (x_i, V, D_i^{vw}) to *n+1*
  7. Update $\overline{U}$ to *n+1*
  8. Update *p* and *c* from EOS

Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

The mesh motion is computed from a physics-based mesh velocity rather than a quality-based mesh relaxer

- Smoothed Lagrangian approach: Set $w_i = u_i$ then iterate on the linear system

$$\nabla^2 (k w_i) = 0 \qquad k = c_1 \max\left(0, 1 - c_2 \frac{\omega_i}{\|\omega_i\|\infty}\right)$$

- Helmholtz approach: Set w_i equal to the irrotational component of u_i as computed from a Helmholtz decomposition

$$u_i = u_{i,rot} + u_{i,irrot} = u_{i,rot} + \frac{\partial \phi}{\partial x_i}$$

The scalar potential is computed from the solution to the Poisson equation

$$\frac{\partial^2 \phi}{\partial x_i^2} = \frac{\partial u_i}{\partial x_i} \rightarrow w_i = \frac{\partial \phi}{\partial x_i}$$

Key features:

1. Mesh velocity is independent of local mesh size
2. Mesh is stationary where the fluid is stationary
3. High-vorticity regions behave more Eulerian
4. Low-vorticity regions behave more Lagrangian

A mesh force model similar to Lagrangian Q models is applied to the mesh velocity for additional robustness

- The mesh velocity at each node *v* is evolved according to

$$w_i^{v,k+1} = u_i^k + \frac{\alpha^k \Delta t}{V^{v,k}} F_i^{v,k}$$

- The pseudo-force F_i is computed as a surface integral of pseudo-pressures (recall that d_i is a surface area normal of a control volume facet)

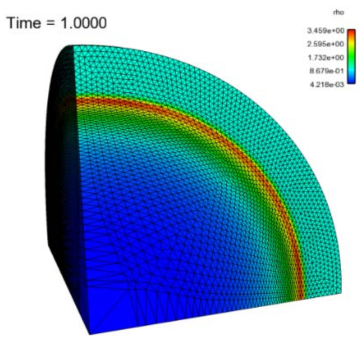
$$F_i^v = \frac{1}{2} \sum_{vw \in v} \sum_{\Omega_h \in vw} d_i^{vw} q^{\Omega}$$

- The pseudo-pressure *q* is computed from VNR- and TQS-like terms

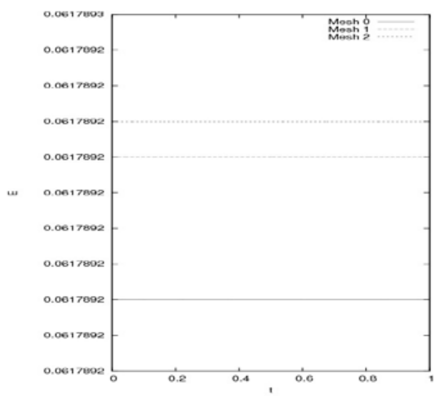
$$q = q^{\Delta u} + q^{\Delta V} = -\rho\left(b_1 c \Delta u + b_2 \Delta u^2\right) - \rho b_3 c^2 \max\left(0, \frac{V^{t=0}}{V^k} - 1\right)$$

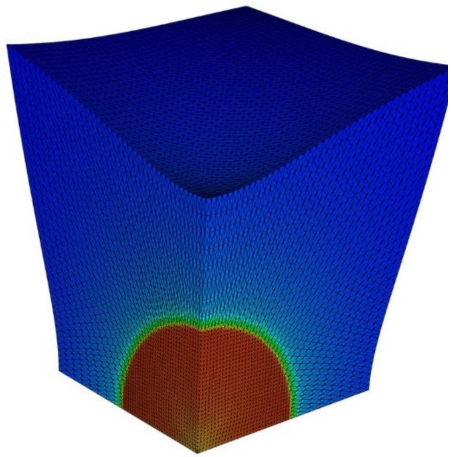
VNR-like term **TQS-like term**

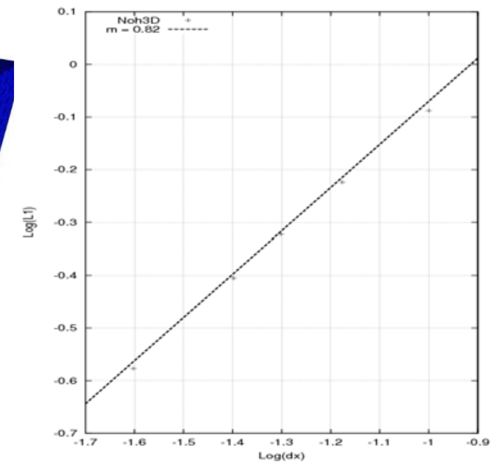
The single-material ALE algorithm has been heavily verified on shock and shock-free problems

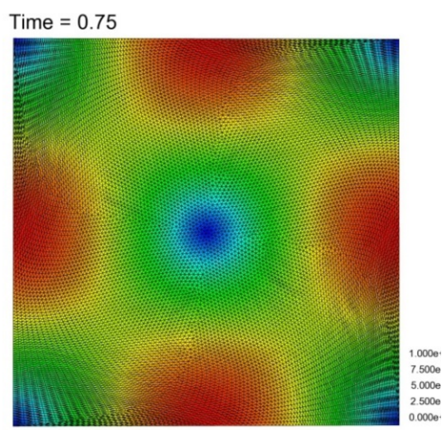


Sedov ALE

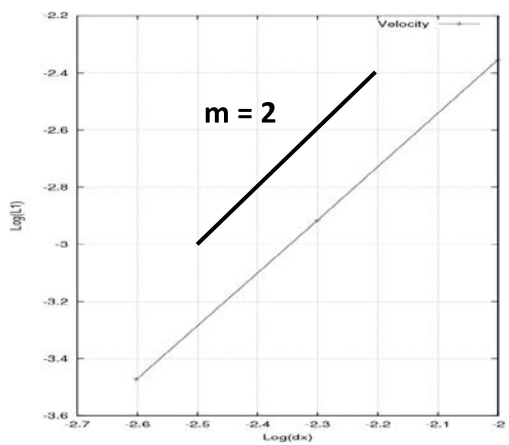


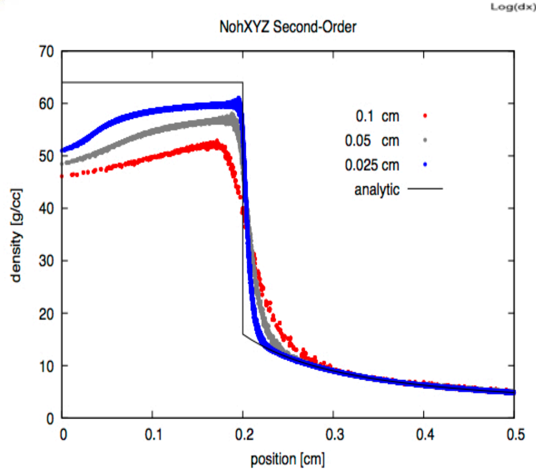






Taylor-Green ALE



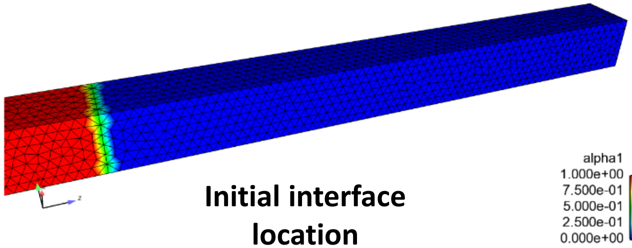


Noh Lagrangian

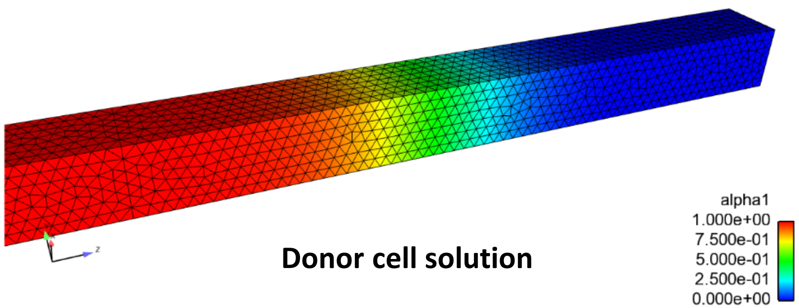
UNCLASSIFIED

The interface equation is initially being solved with a SuperBee limiter and Godunov flux

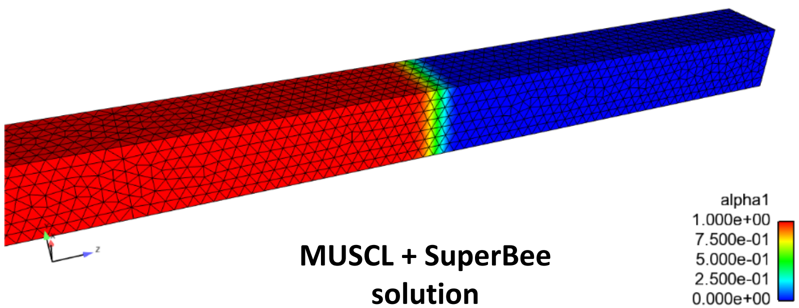
- Interface advection test problem (Eulerian)
  - Two materials, same state, constant u_i



Initial interface location



Donor cell solution

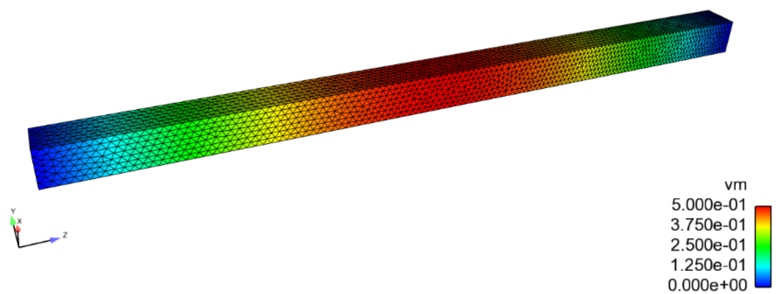


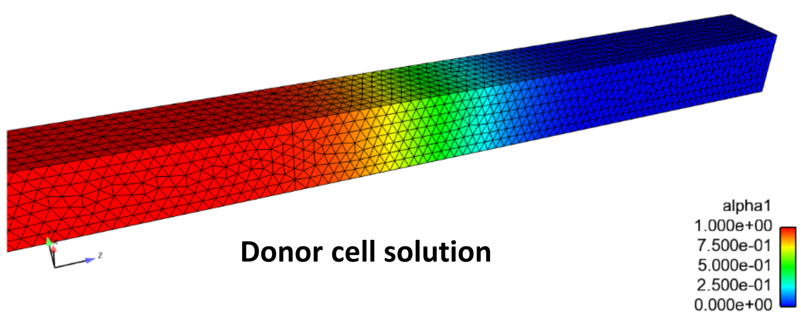
MUSCL + SuperBee solution

- The Hyper C compressive limiter also is being tested
  - Caveat: the limit of zero numerical diffusion is perfect mesh imprinting! May not be the best choice on highly unstructured grids…

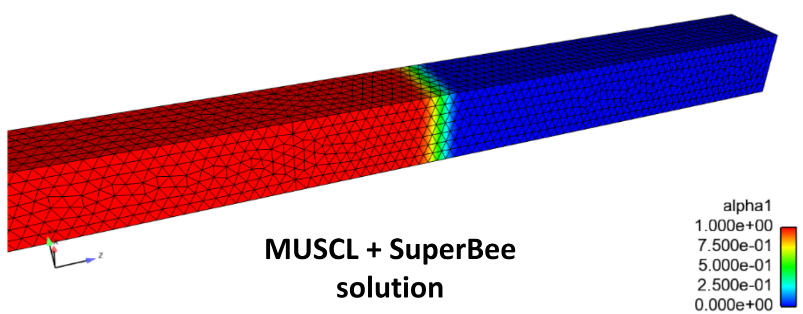
Similar results are obtained with ALE using a prescribed mesh velocity

- Interface advection test problem (ALE)
  - Sinusoidal mesh velocity along the length of the domain





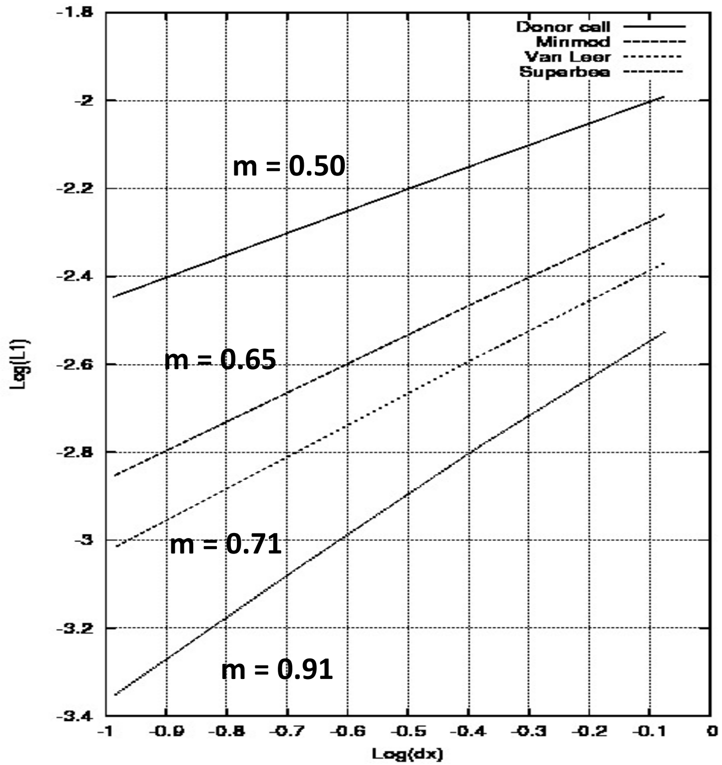
Donor cell solution

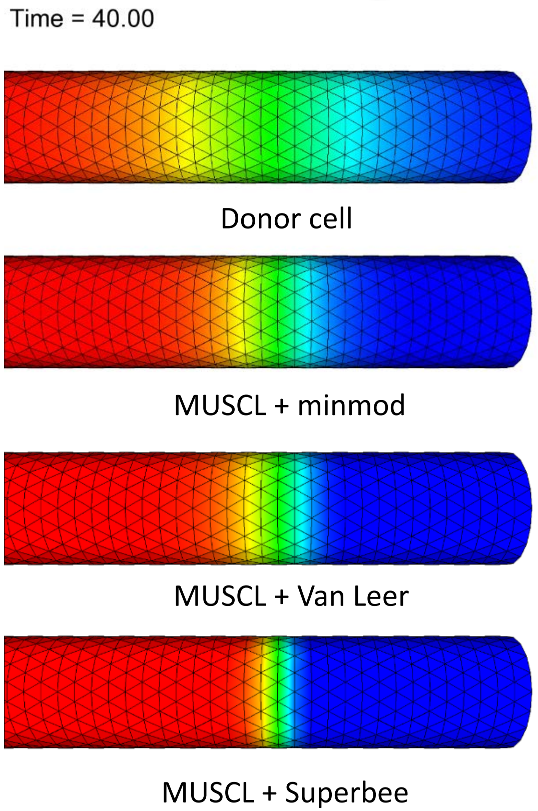


MUSCL + SuperBee solution

The SuperBee limiter obtains much closer to first-order convergence compared to other limiters

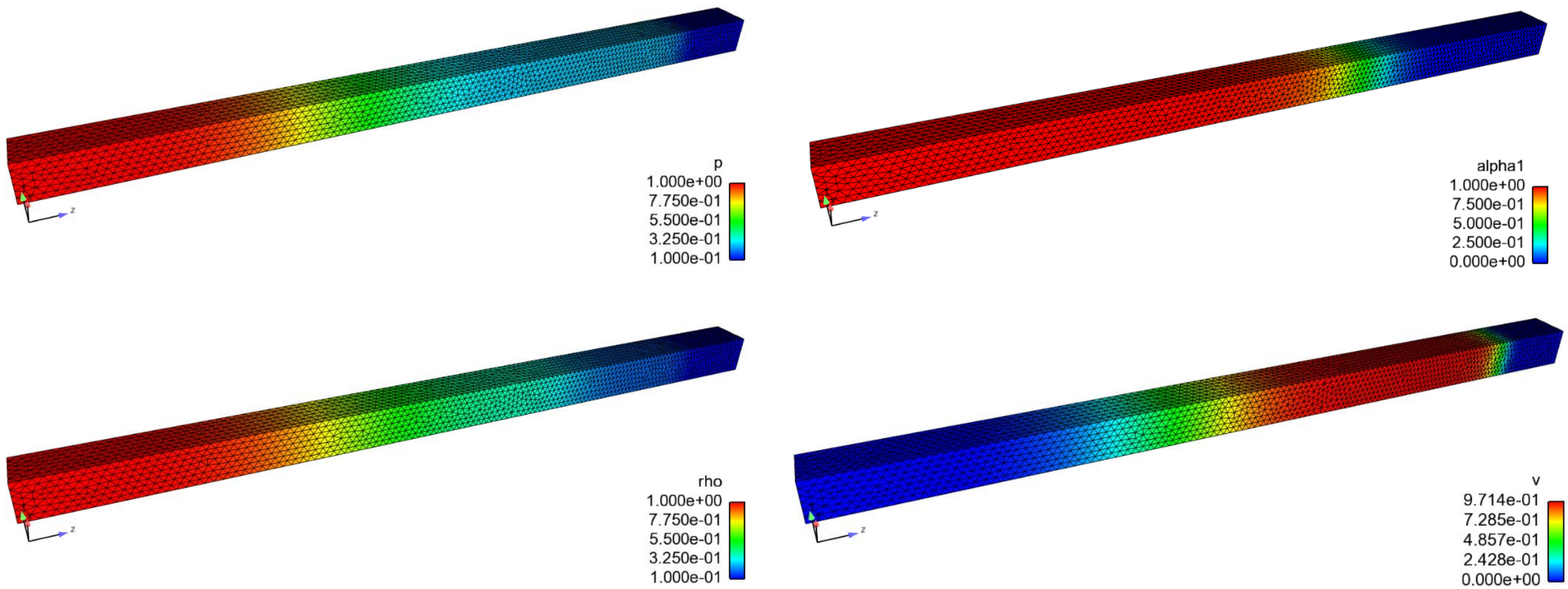
- Eulerian advection test + convergence study





Initial donor cell results have been obtained on the shock tube problem

- Results are qualitatively correct (and diffuse as expected)
  - Smoothed Lagrangian mesh velocity



UNCLASSIFIED

A direct ALE method for multi-material flows on unstructured grids is under development

- Based on the generalization of a single-material Godunov scheme to multiple materials
- Key features
  - Direct solution of the multi-material ALE hydro equations
  - Approximate Riemann solvers in moving reference frame
  - Mesh velocity based on local fluid velocity with smoothing
  - Algebraic treatment of volume fraction equation
- Preliminary results on initial test problems have been obtained
  - Multiple interface methods under investigation
  - Further testing/validation is in progress