Constrained optimization framework for interface-aware sub-scale-dynamics closure models for multi-material cells in Arbitrary-Lagrangian-Eulerian Hydrodynamics

Mikhail Shashkov

XCP-4, Methods & Algorithms Group, LANL, USA

shashkov@lanl.gov

webpage: cnls.lanl.gov/∼ shashkov

Andrew Barlow

AWE Aldermaston, England, UK

Ryan Hill

XCP-4, LANL, USA

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Motivation

Multi-material Arbitrary Lagrangian-Eulerian Methods

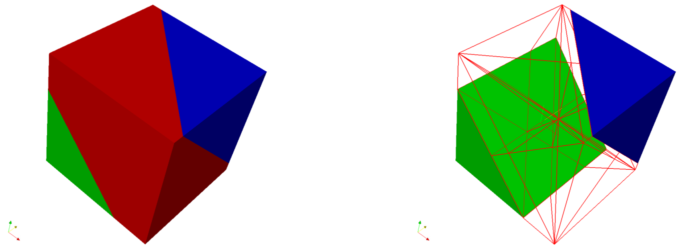
- Explicit Lagrangian (solving Lagrangian equations) phase — grid is moving with fluid
- Rezone phase — changing the mesh (improving geometrical quality, smoothing, adaptation)
- Remap phase - data transfer from Lagrangian grid to rezoned mesh
- Material interfaces may not coincide with mesh faces even for pure Lagrangian calculation - complicated shapes, painting
- Multi-material cells - cells which contain more than one material - distinct interface between materials

Multi-material Lagrangian Hydro - Closure models

- Staggered Hydro - single velocity for all materials - one velocity per node
- Each material has its own mass (volume,density), internal energy, and pressure
- Each cell (including multi-material cell) has to produce one force to its vertices - one pressure to be used in momentum equation

Closure model for multi-material cell

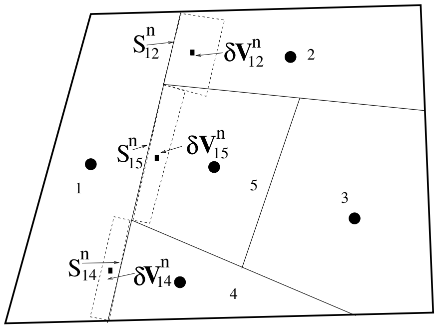
- How to advance in time volume (density) and internal energy for each material and
- How to produce force from multi-material cell to its nodes



Types of - Closure models

- **Pressure Equilibrium (Pressure Relaxation) - Explicitly Enforced**
  - **Example - Tipton's (LLNL) model - does NOT require knowledge of interfaces between materials in the multi-material cell**

- **Modeling Sub-scale Dynamics**
  - **Models interaction of materials inside multi-material cell**
  - **Requires information about material interfaces inside multi-material cell - interface reconstruction (Moment-of-Fluid)**



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Tipton's Pressure Relaxation Model
R. Tipton (LLNL) - unpublished notes, 1989

Pressure relaxation model

$$p_i^{n+1/2} + R_i^{n+1/2} = p^{n+1/2}\,,\; i - \textbf{material index}\,,\; R_i^{n+1/2} - \textbf{relaxation term}$$

Relaxation term resembles viscosity

$$R_i = -l_i\,\rho_i\,(\mathbf{div}\,\mathbf{u})_i\,,\;(\mathbf{div}\,\mathbf{u})_i = (1/V_i)\,(dV_i/dt)$$

$$R_i^{n+1/2} = -L^n\,\rho_i^n\,c_i^n\,(1/V_i^n)\,(\delta V_i^{n+1/2}/\delta t)$$

Assumption - Isentropic: $dS_i/dt = 0$

$$p_i^{n+1/2} = p_i^n - \rho_i^n\,(c_i^n)^2\,\delta V_i^{n+1/2}/V_i^n$$

Closure Model

$$p_i^n - \rho_i^n\,(c_i^n)^2\,[1 + L^n/(c_i^n\delta t)]\delta V_i^{n+1/2}/V_i^n = p^{n+1/2}\,,\quad \sum_i \delta V_i^{n+1/2} = \delta V^{n+1/2}$$

Explicit solution

$$p^{n+1/2} = \bar{p}^n - \bar{B}^n \, \delta V^{n+1/2} / V^n$$

$$\delta V_i^{n+1/2} = \left(\frac{f_i^n}{B_i^n} \, \bar{B}^n \right) \delta V^{n+1/2} + \frac{V_i^n}{B_i^n} \left(p_i^n - \bar{p}^n \right)$$

where

$$B_i^n = \rho_i^n \left(c_i^n \right)^2 \left[1 + L^n / (c_i^n \delta t) \right], \, \bar{B}^n = 1 \bigg/ \left(\sum_i \frac{f_i^n}{B_i^n} \right)$$

$$\bar{p}^n = \sum_i \left(\frac{f_i^n}{B_i^n} \, p_i^n \right) \bigg/ \sum_i \frac{f_i^n}{B_i^n}$$

Bulk update - distribution of $\delta V^{n+1/2}$ between materials:

Coefficients $\beta_i = \frac{f_i^n}{B_i^n} \, \bar{B}^n$ **are dimensionless,** $\sum_i \beta_i = 1$

Internal dynamics - taking into account difference in pressures $\sim (p_i^n - \bar{p}^n)$**:**

Coefficients $\frac{V_i^n}{B_i^n}$ **has following dimension** $\frac{Length^2 \times Time}{Density \times Velocity}$

Parameters: L^n **- controls relaxation; maximum change in volume fractions** $\sim 25\%$

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Interface-aware sub-scale dynamics closure model

Modeling interaction of materials inside multi-material cell

Material volume update

- **Bulk update - equal volumetric strain (constant volume fraction)**

$$V_i^{bulk,n+1} = f_i^n \, V^{n+1} \quad \rightarrow \quad \Delta V_i^{bulk,n+1} = f_i^n \, \Delta V^{n+1}$$

- **Sub-scale dynamics - interaction of the materials inside multi-material cell**

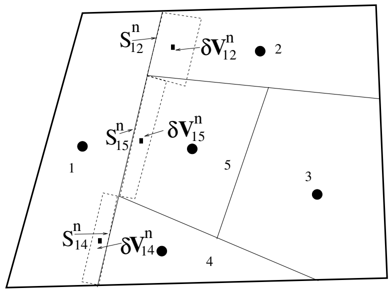
$$\Delta V_i^{n+1} = \Delta V_i^{bulk,n+1} + \sum_{k \in M(i)} \delta V_{i,k} \,, \quad \delta V_{i,k} = -\delta V_{k,i}$$

Interface-aware sub-scale dynamics closure model

Material volume update

$$\delta V_{i,k} = \Psi_{i,k}\,\delta V_{i,k}^{max}\,, \quad \Psi_{i,k} \in [0,1]$$ – **is a limiter**

Maximum volume exchanges are estimated from an acoustic Riemann solver



$$\delta V_{i,k}^{max} = \frac{p_i - p_k}{\rho_i\, c_i + \rho_k\, c_k} S_{i,k}\, dt$$

Requirement $V^{n+1} > V_i^{n+1} > 0$

Goal it to find $\Psi_{i,k}$ as close as possible to 1 such that this requirement is satisfied

This can be formulated as quadratic optimization problem with linear constraints

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Interface-aware sub-scale dynamics closure model

Material volume update

We will require

$$V_i^{n+1} \geq \alpha_{bot} V_i^{bulk,n+1} = \alpha_{bot} f_i^n V_i^{n+1} > 0\,, \quad 1 \geq \alpha_{bot} > 0$$

This inequality is always satisfied when all $\Psi_{i,k} = 0$ - in this case $V_i^{n+1} = V_i^{bulk,n+1}$

Also, because $V_i^{n+1} > 0$ we have

$$V_{i_0} = V_{n+1} - \sum_{i \neq i_0} V_i^{n+1} < V^{n+1}$$

Feasible set for optimization problem is not empty

Interface-aware sub-scale dynamics closure model

Internal energy update

Each material has its own $p\,dV$ equation

$$m_i\,(\varepsilon_i^{n+1} - \varepsilon_i^n) \sim -p_i^n\,\Delta V_i^{n+1}$$

Conservative form

$$m_i\,(\varepsilon_i^{n+1} - \varepsilon_i^n) = -p_i^n\,\Delta V_i^{bulk,n+1} - \sum_{k\in M(i)} p_{i,k}^*\,\Psi_{i,k}\,\delta V_{i,k}^{max}$$

Interfacial pressure $p_{i,k}^*$ is estimated from acoustic Riemann solver

$$p_{i,k}^* = \frac{\kappa_k\,p_i + \kappa_i\,p_k}{\kappa_i + \kappa_k} - \frac{\kappa_i\,\kappa_k}{\kappa_i + \kappa_k}\,(\mathbf{n}_{i,k}\cdot(\mathbf{u}_k - \mathbf{u}_i))\ , \quad \kappa = \rho\,c$$

$\mathbf{n}_{i,k}$ **- unit normal to interface between materials i and k**

$\mathbf{u}_i\ ,\ \mathbf{u}_k$ **- velocity of the materials**

Interface-aware sub-scale dynamics closure model
Internal energy update

Requirement - $\varepsilon_i^{n+1} > 0$

Assumption (equal volumetric strain produces positive internal energy) $\sim$ **constraint on** dt **which does not depend on volume fraction**

$$m_i\, \varepsilon_i^{bulk,n+1} = m_i\, \varepsilon_i^n - p_i^n\, \Delta V_i^{bulk,n+1} > 0$$

$$\Delta V^{n+1}/V_n < 1/(\gamma_i - 1) \sim dt < 1/((\gamma_i - 1)\, \mathbf{DIV}\ \mathbf{u})$$

Under this assumption the Requirement - $\varepsilon_i^{n+1} > 0$ **leads to another system of linear constraints**

$$\sum_{k \in M(i)} p_{i,k}^{*}\, \Psi_{i,k}\, \delta V_{i,k}^{max} \leq m_i\, \varepsilon_i^{bulk,n+1}$$

for $\Psi_{i,k}$

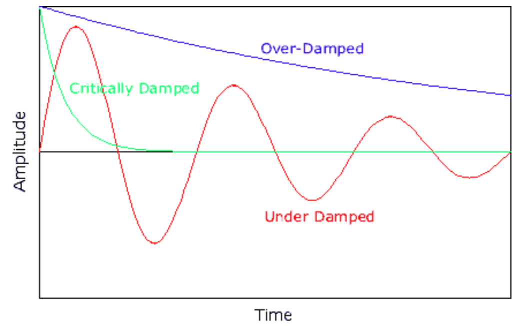
Interface-aware sub-scale dynamics closure model

Smooth pressure relaxation - ”stability”

Design principles

- **Sub-scale model has to bring pressures obtained from bulk update closer to each other**

- **During relaxation material pressures not suppose to overshoot each other - critical damping idea (analogy with damped harmonic oscillator)**



Interface-aware sub-scale dynamics closure model

Smooth pressure relaxation - stability

- **The approximate ($dS_i/dt = 0$) pressure update is**

$$p_i^{n+1} = p_i^{bulk,n+1} - \frac{\rho_i^n (c_i^n)^2}{V_i^n} \sum_{k \in M(i)} \Psi_{i,k} \delta V_{i,k}^{max} , \quad p_i^{bulk,n+1} = p_i^n - \frac{\rho_i^n (c_i^n)^2}{V_i^n} \Delta V_i^{bulk,n+1}$$

- **Temporary equilibrium pressure, toward which the material pressures has to relax**

$$\bar{p} = \sum_i f_i^n \, p_i^{bulk,n+1}$$

- **If $p_i^{bulk,n+1} \geq \bar{p}$ - we require $\alpha_i \, \bar{p} + (1 - \alpha_i) \, p_i^{bulk,n+1} \leq p_i^{n+1} \leq p_i^{bulk,n+1}$**
- **If $p_i^{bulk,n+1} \leq \bar{p}$ - we require $\alpha_i \, \bar{p} + (1 - \alpha_i) \, p_i^{bulk,n+1} \geq p_i^{n+1} \geq p_i^{bulk,n+1}$**
- $1 > \alpha_i > 0$ **- parameter to control the rate of the equilibration**

Additional system of linear inequalities for $\Psi_{i,k}$

Interface-aware sub-scale dynamics closure model
Constrained optimization framework

- **Quadratic objective function -** $\sum_i \sum_{k \in M(i)} (1 - \Psi_{i,k})^2$

- **System of linear constraints for** $\Psi_{i,k}$
  - $1 \geq \Psi_{i,k} \geq 0$
  - **Positivity of material volumes**
  - **Positivity of internal energy**
  - **Controlled equilibration of the material pressures**

- **Software**
  - **QL: A Fortran Code for convex quadratic programming - User's Guide, February, 2011**
    K. Schittowski - www.klaus-schittkowski.de/software.htm
  - **MOF - Moment-of-Fluid Interface Reconstruction**

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Two-materials - Explicit Solution

- **Volume constraints**
  - $\delta V_{12}^{max} > 0 \quad \rightarrow 0 \leq \Psi_{12} \leq \frac{1-\alpha_{bot}}{|\delta V_{12}^{max}|} V_2^{bulk,n+1}$
  - $\delta V_{12}^{max} < 0 \quad \rightarrow 0 \leq \Psi_{12} \leq \frac{1-\alpha_{bot}}{|\delta V_{12}^{max}|} V_1^{bulk,n+1}$

- **Internal energy constraints**
  - $\delta V_{12}^{max} > 0 \quad \rightarrow 0 \leq \Psi_{12} \leq m_1 \, \varepsilon_1^{bulk,n+1} \Big/ |p_{12}^* \, \delta V_{12}^{max}|$
  - $\delta V_{12}^{max} < 0 \quad \rightarrow 0 \leq \Psi_{12} \leq m_2 \, \varepsilon_2^{bulk,n+1} \Big/ |p_{12}^* \, \delta V_{12}^{max}|$

- **Pressure equilibration constraints**
  - $0 \leq \Psi_{12} \leq \min \left(\frac{(1-\alpha_1) \, |p_1^{bulk,n+1} - \bar{p}|}{\rho_1^n \, (c_1^n)^2 \, |\delta V_{12}^{max}|}, \frac{(1-\alpha_2) \, |p_2^{bulk,n+1} - \bar{p}|}{\rho_2^n \, (c_2^n)^2 \, |\delta V_{12}^{max}|} \right)$

Numerical Experiments - 1D
Water-Air Riemann Problem

A. Murrone and H. Guillard, JCP, 202 (2005), p. 664

Statement of the problem

$p = (\gamma - 1)\,\rho\,\varepsilon - \gamma\,\pi$ | $p = (\gamma - 1)\,\rho\,\varepsilon$

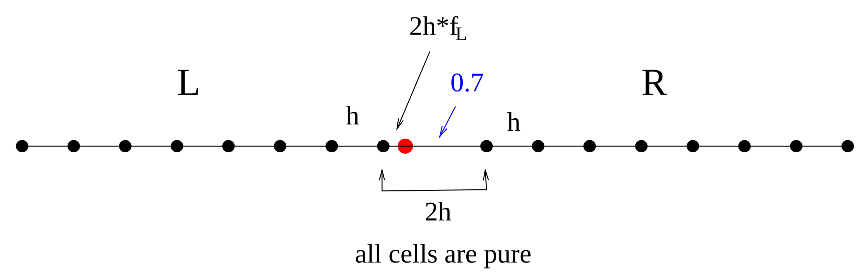
$\gamma = 4.4,\ \pi = 6 * 10^8$ | $\gamma = 1.4$

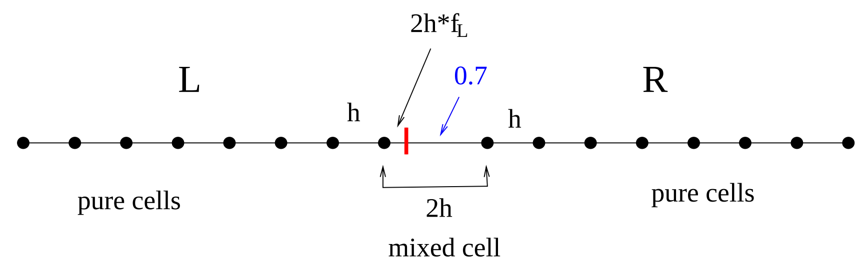
$p = 10^9,\ \rho = 10^3$ | $p = 10^5,\ \rho = 50$

$u = 0$ | $u = 0$

$t = 2.29 * 10^{-4}$

1000 cells

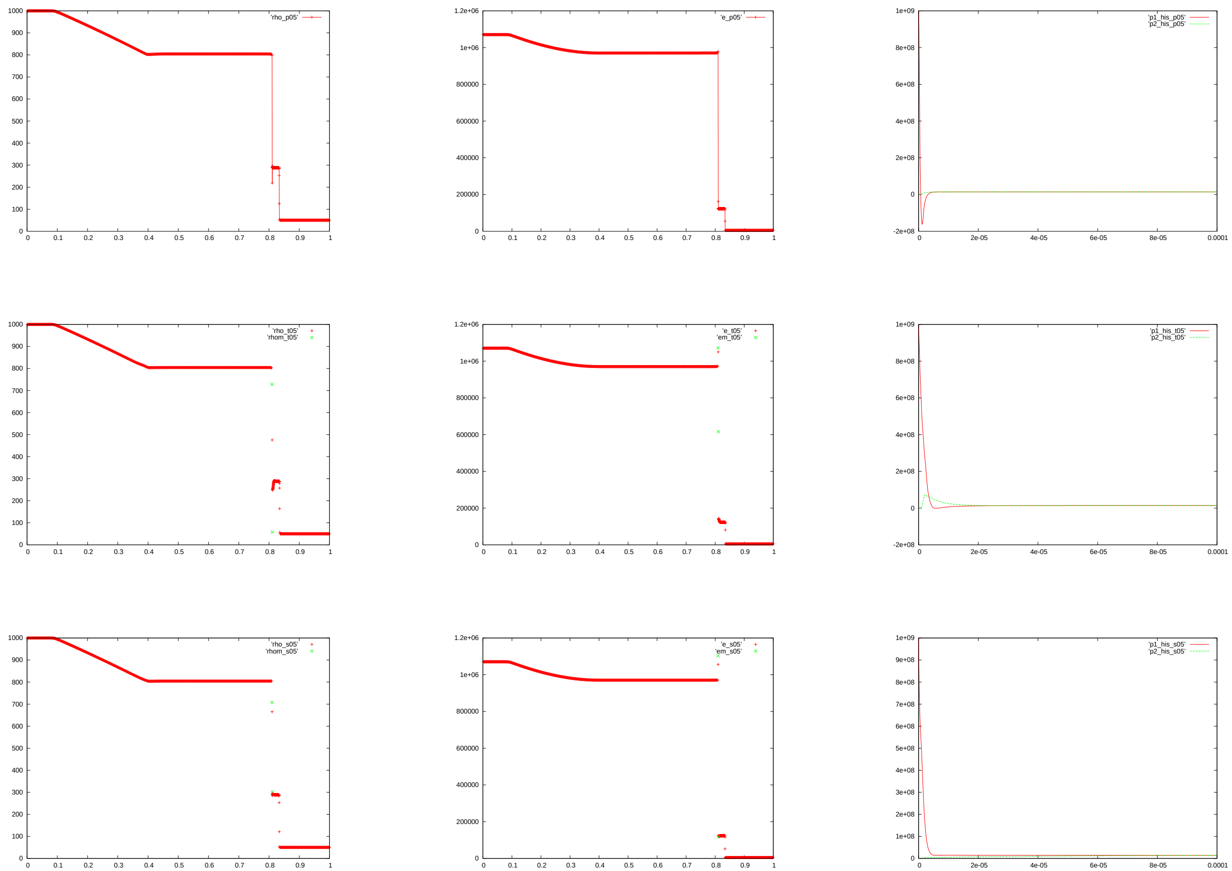




999 cells

Numerical Experiments - 1D
Water-Air Riemann Problem - $f_L = 0.5$

Pure - Top, Tipton - Middle, IA-SSD - Bottom

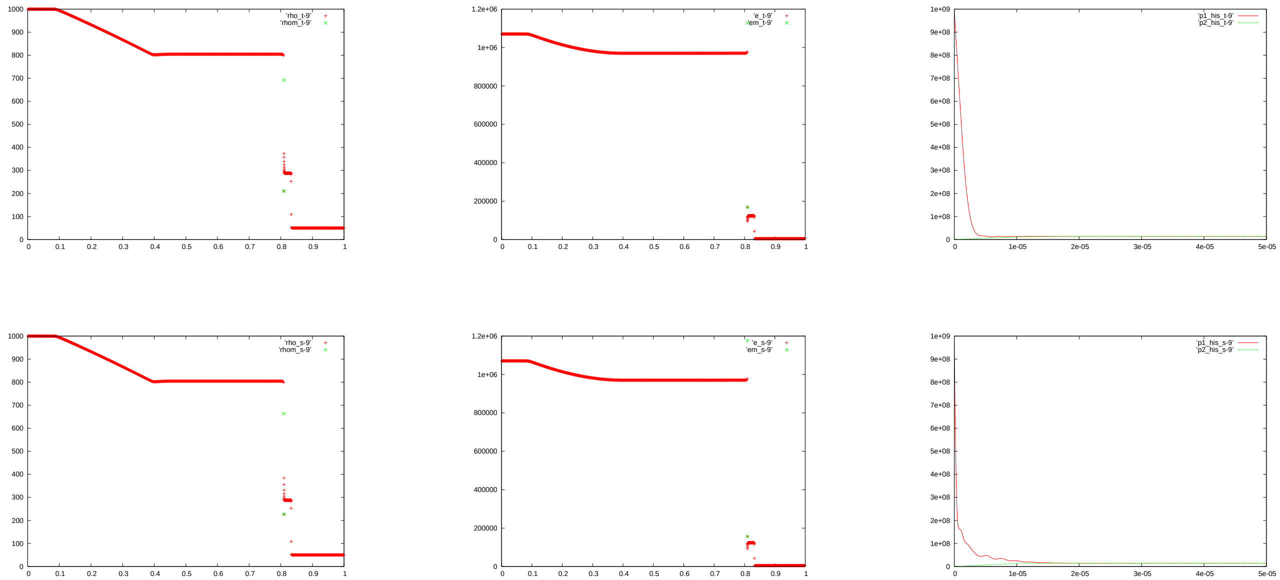


Density **Internal Energy** **Pressure History**

Numerical Experiments - 1D
Water-Air Riemann Problem - $f_L = 10^{-9}$

Tipton - Top, IA-SSD - Bottom

- **Pure cell calculations are not feasible - small dt**
- **Tipton's model runs with standard $L = mixed\ cell\ size$**



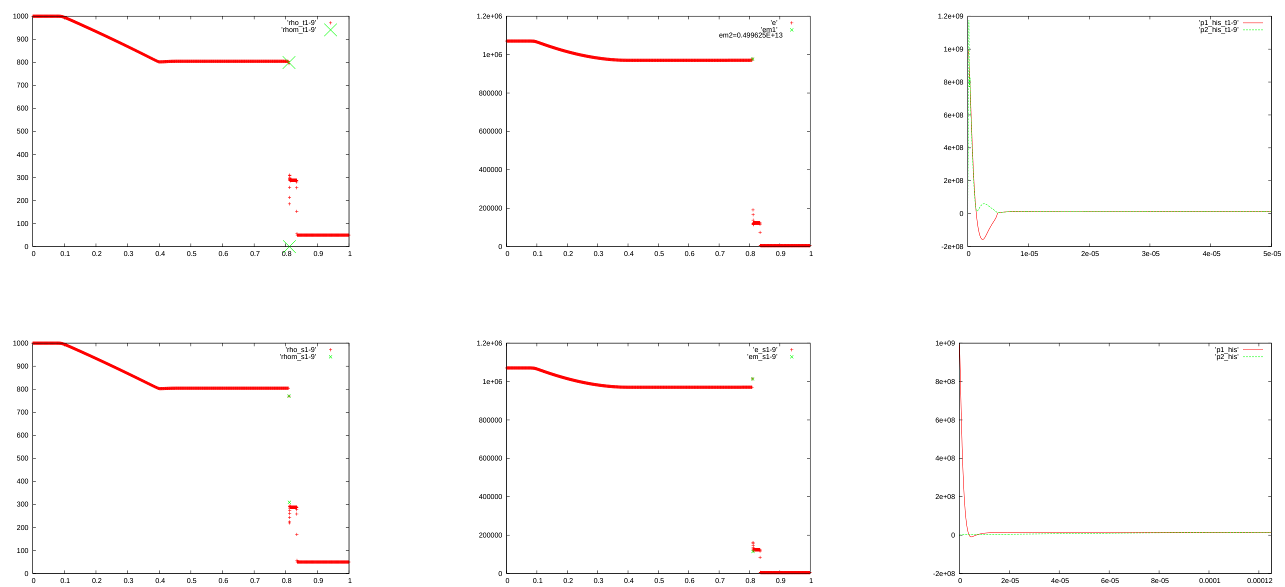
Density **Internal Energy** **Pressure History**

Numerical Experiments - 1D

Water-Air Riemann Problem - $f_L = 1 - 10^{-9}$

Tipton - Top, IA-SSD - Bottom

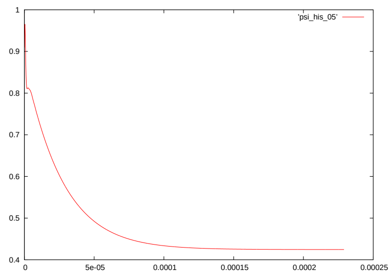
- **Pure cell calculations are not feasible - small dt**
- **Tipton's model only runs for very small L - no relaxation, and produces internal energy in the materials in the multi-material cells, which are absolutely out of range and reverse - $e_2 = 0.49 \cdot 10^{13}$**
- **We were not able to find any parameters (relaxation parameter, bounds for change in volume fractions) for Tipton's model which will produce reasonable material energies in the multi-material cell.**



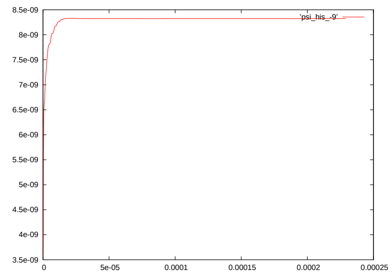
Density **Internal Energy** **Pressure History**

Numerical Experiments - 1D
Water-Air Riemann Problem

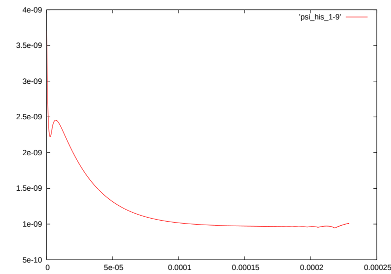
Time History for Limiter for IA-SSD Model for Different Initial Volume Fractions



$f_L = 0.5$



$f_L = 10^{-9}$

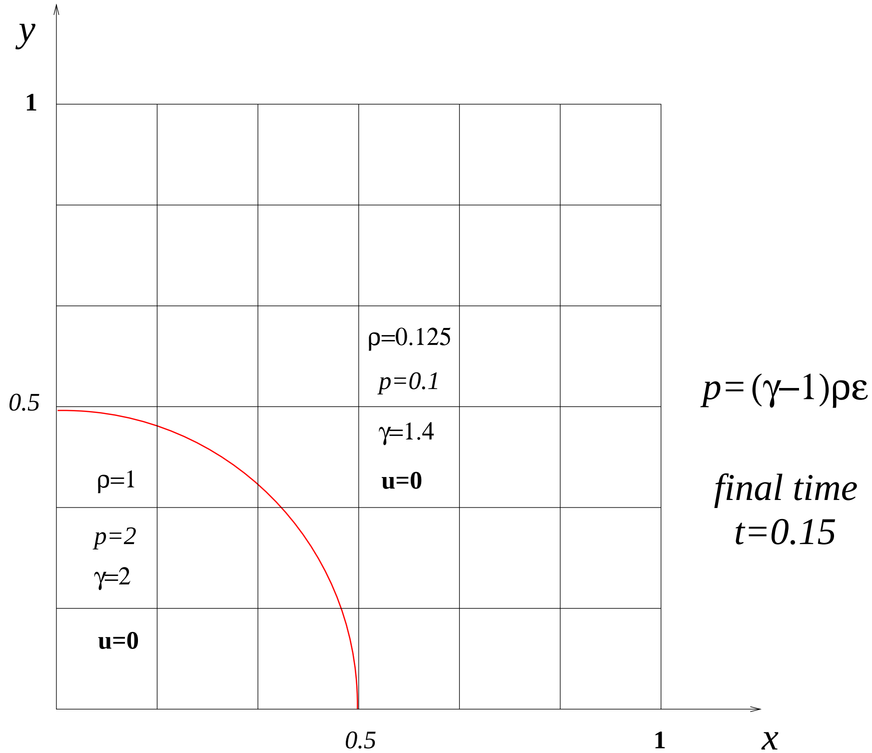


$f_L = 1 - 10^{-9}$

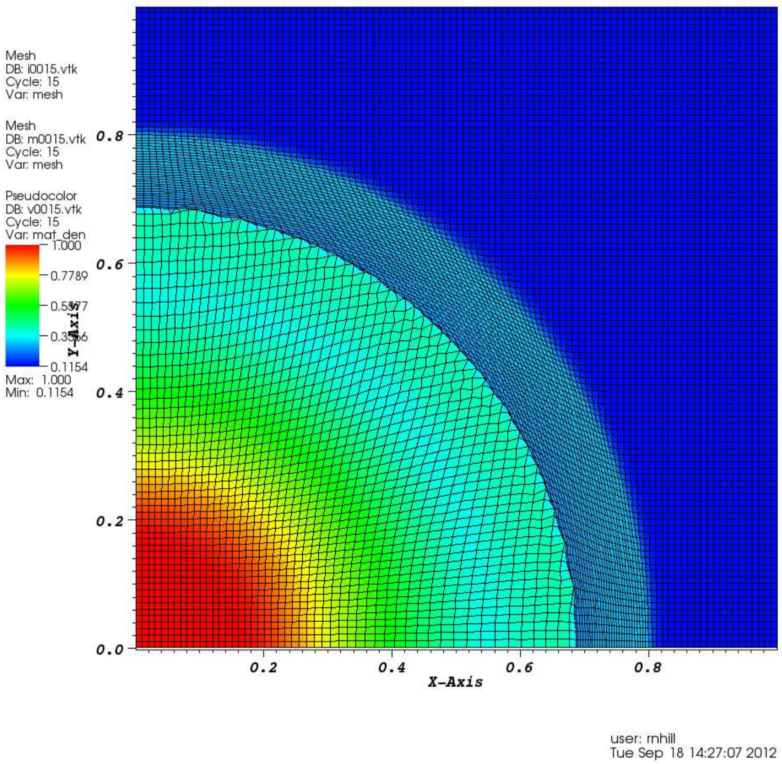
NO USER INTERVENTION - SAME SETTINGS for ALL CASES

Numerical Experiments
2D Radial Sod Problem - Initial Square Mesh

Lagrangian Calculations with Multi-material Cells



Statement of the problem



Mesh and density at the final time

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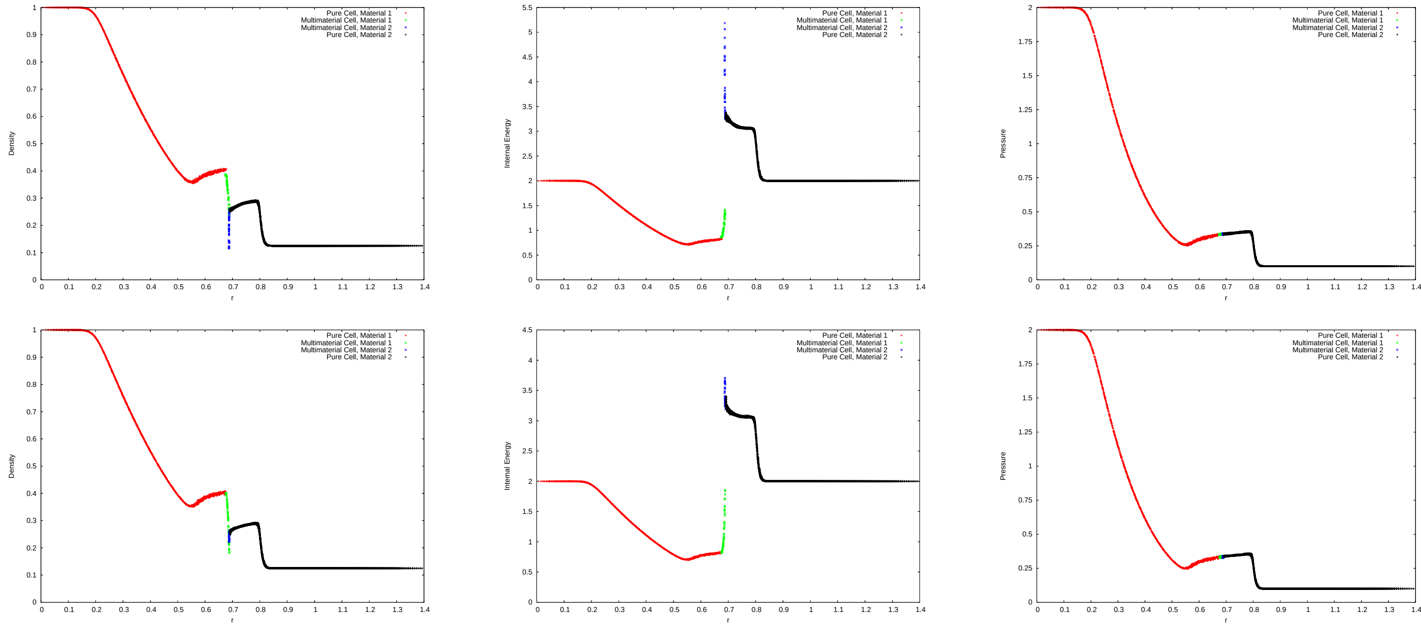
Numerical Experiments
2D Radial Sod Problem

Scatter Plots: Top - Tipton, Bottom - IA-SSD

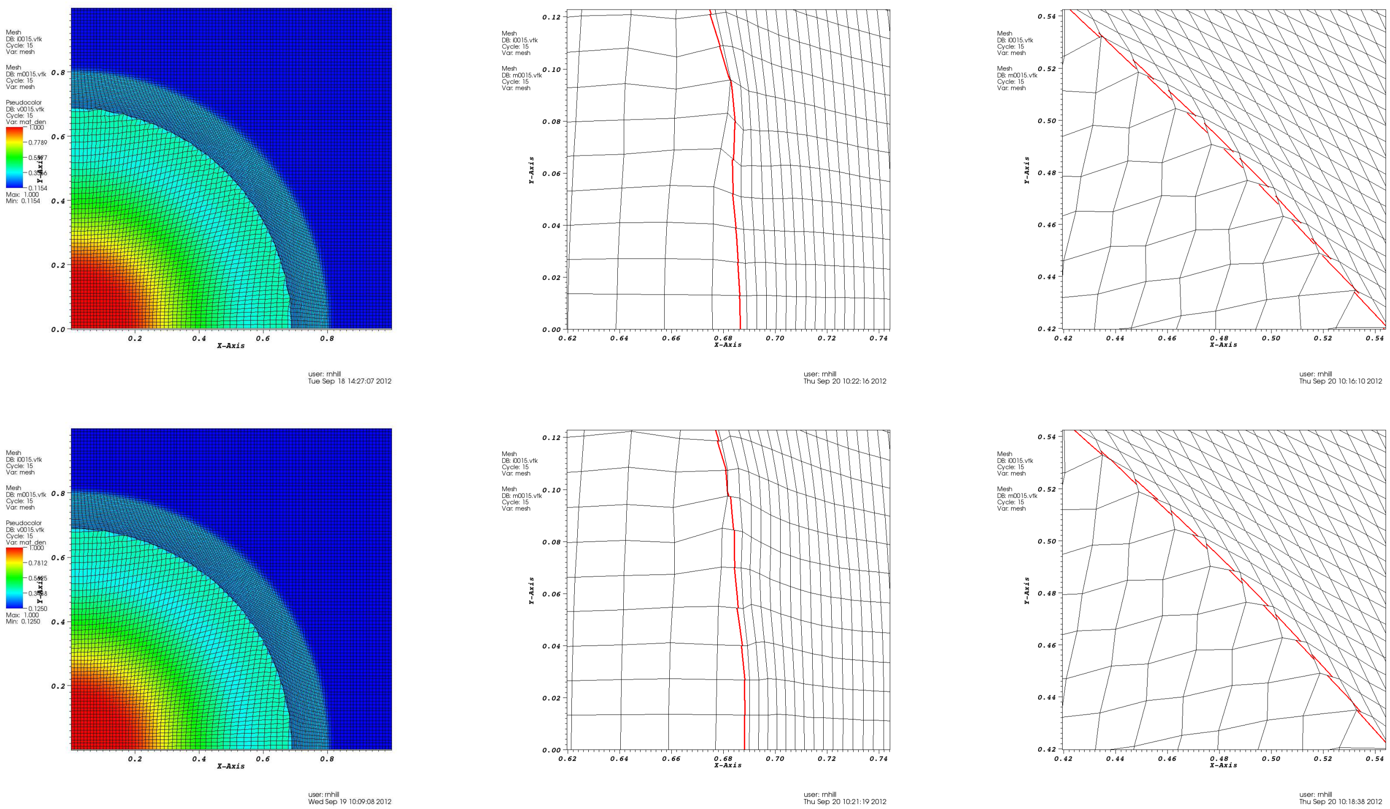


Density **Internal Energy** **Pressure**

Red - Mat. 1 in pure cells; Green- Mat. 1 in MM. cells; Blue- Mat. 2 in MM. cells; Black- Mat. 2 in pure cells;

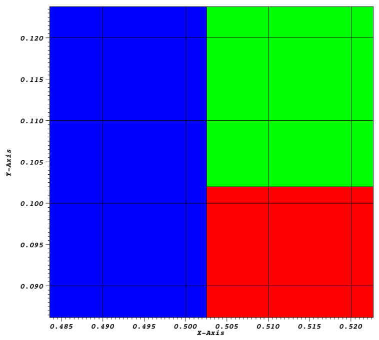
Numerical Experiments
2D Radial Sod Problem
Fragments of the Mesh with Interfaces in Multi-material Cells

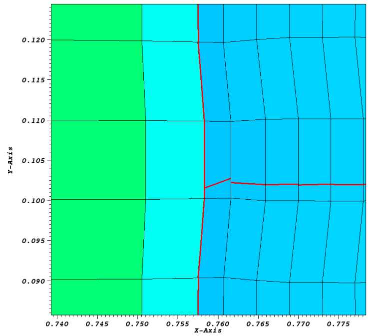
Top - Tipton, Bottom - IA-SSD



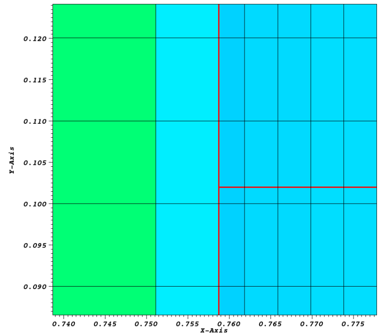
Entire Mesh | **Zoom - Close to x axis** | **Zoom - Close to 45° line**

Modified Sod Problem. Three material cell with T-junction and symmetry preservation





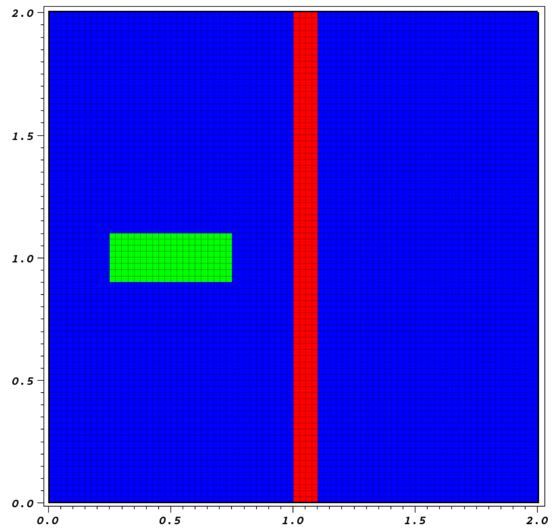
Tipton



IA-SSD

Interface positions at $t = 0.2$, modified Sod problem, 2D calculation, non-symmetric 'T'-junction case

Impact Problem - Robustness Test



Green material - the high density gas has properties $\rho_2 = 20.0, p_2 = 2.0, \gamma_2 = 50.0, u = 0.2$ and $v = 0$,

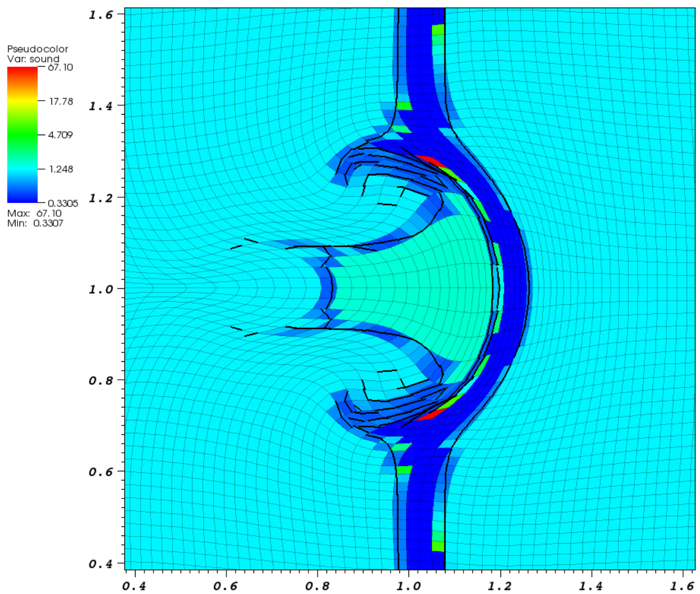
Blue material - (Air) - $\rho_1 = 1.0, p_1 = 1.0, \gamma_1 = 1.4, u = 0$ and $v = 0$,

Red material - the medium density gas has properties $\rho_3 = 15.0, p_3 = 1.0, \gamma_3 = 5/3, u = 0$ and $v = 0$.

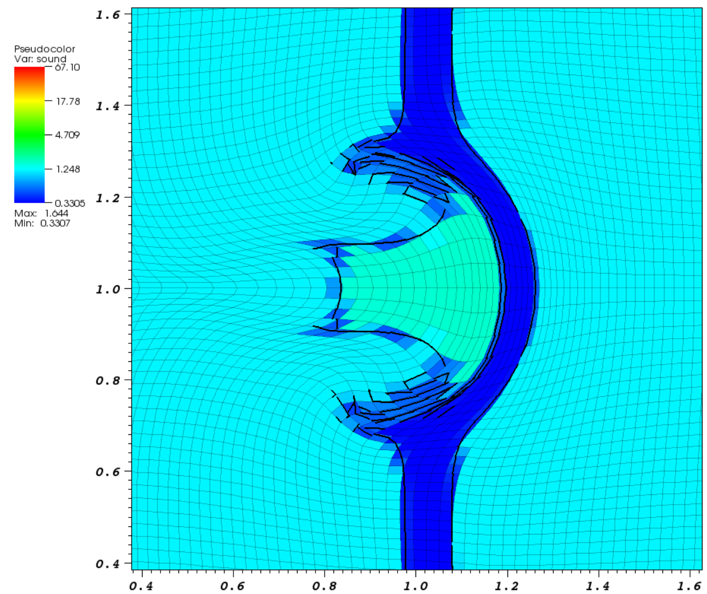
The simulation final time is $t = 8.0$ - 80×80 cells.

ALE-10 regime: a single iteration of the Winslow algorithm to retain the Lagrangian mesh as much as possible

Impact Problem - Robustness Test



Tipton



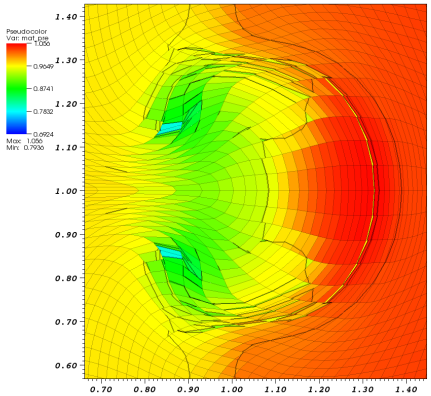
IA-SSD

Sound speed values (logarithm scale) for the impact test case at $t = 3.0$. Note also that the IA-SSD simulation shows less initial break up of material, possibly due to the improved material centroid update that is available.

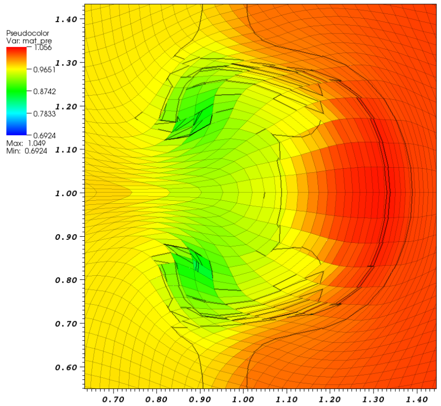
Impact Problem - Robustness Test

The general behavior of the two simulations tend to appear similar, significant differences between the two solutions are apparent

Material pressure values for the impact test case at $t = 4.25$



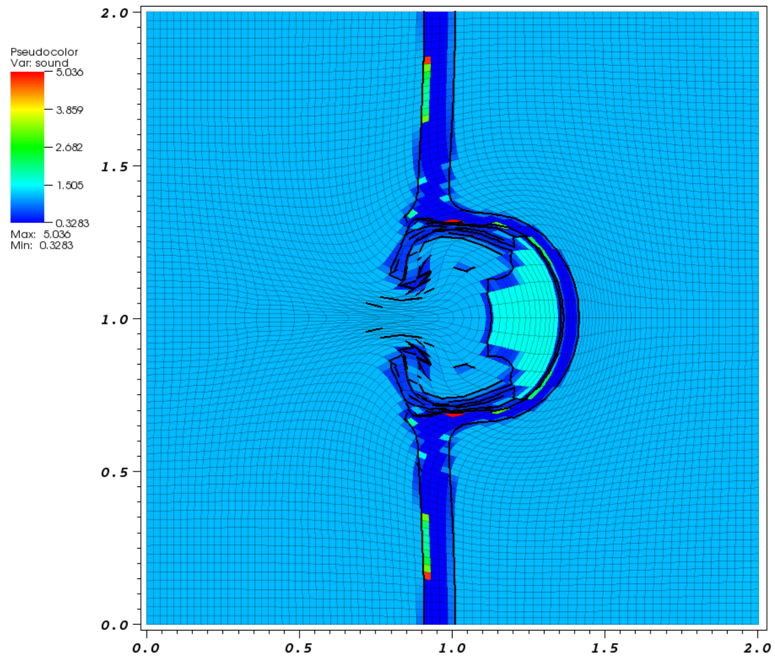
Tipton



IA-SSD

The pressure the air compressed between the high- and medium-density materials differs greatly between methods. The IA-SSD approach achieves equilibrium in all materials, whereas the Tipton solution results in a low pressure for the air. Additionally, the Tipton pressure at the vortices following the impact is also differs from the IA-SSD pressures in the same locations.

Impact Problem - Robustness Test



Cell sound speed values for the Tipton simulation of the impact test case at $t = 4.4705$

just prior to simulation failure

The improved robustness afforded by the IA-SSD approach allows the simulation to run until completion at $t = 8$

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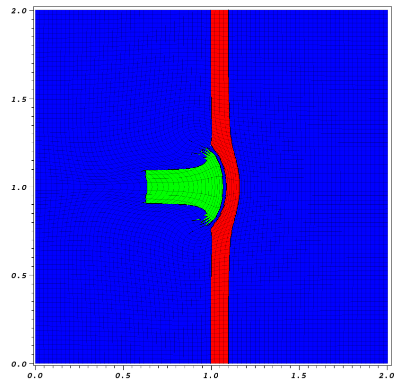
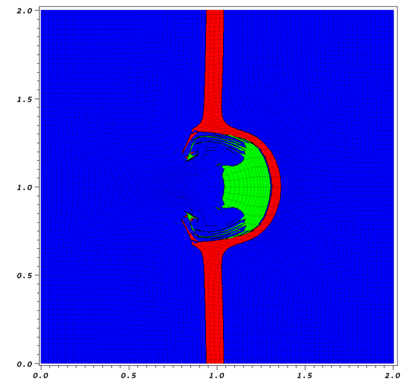
Impact Problem - Robustness Test

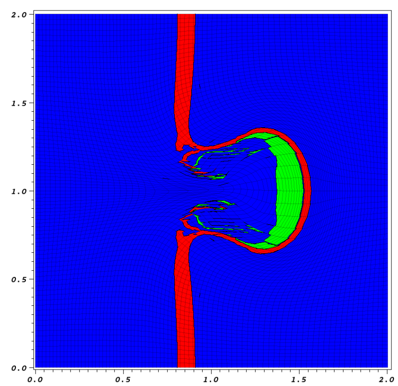
Dynamics of the IA-SSD simulation



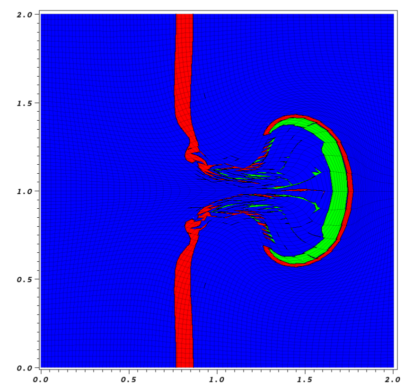
$t = 0.2$



$t = 0.4$



$t = 0.6$



$t = 0.8$

Conclusion and Future Work

- New optimization-based interface-aware subscale dynamics approach to closure models
- No user intervention
- Voids - see poster
- Solids
- Other Physics