Further developments of an interface aware sub-scale-dynamics closure model for multi-material cells

MULTIMAT

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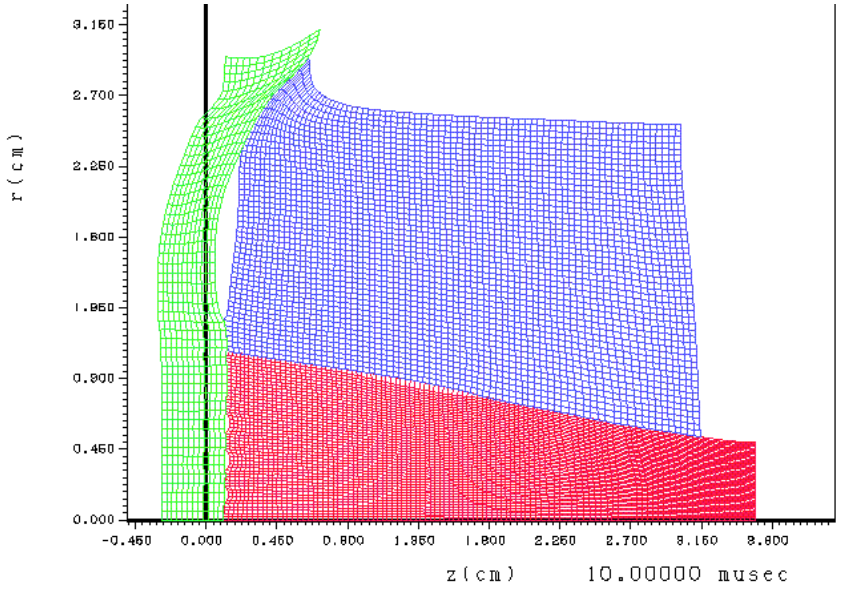
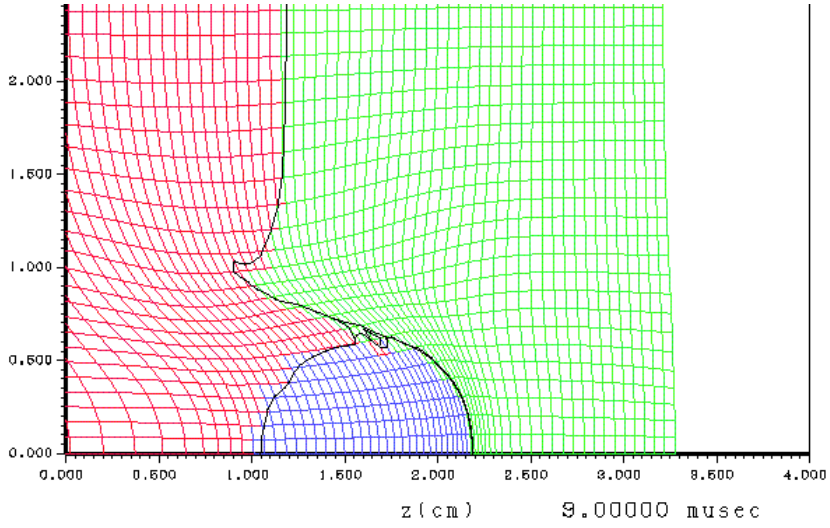
Motivation

- Aim to improve interface physics in multimaterial cells using IA-SSD towards what can be achieved with slide lines
- Overview of IA-SSD will be given emphasising
  - Simplifications to interface aware sub-cell (IA-SSD) dynamics
  - Extension to include voids
- Results will be presented demonstrating performance of method

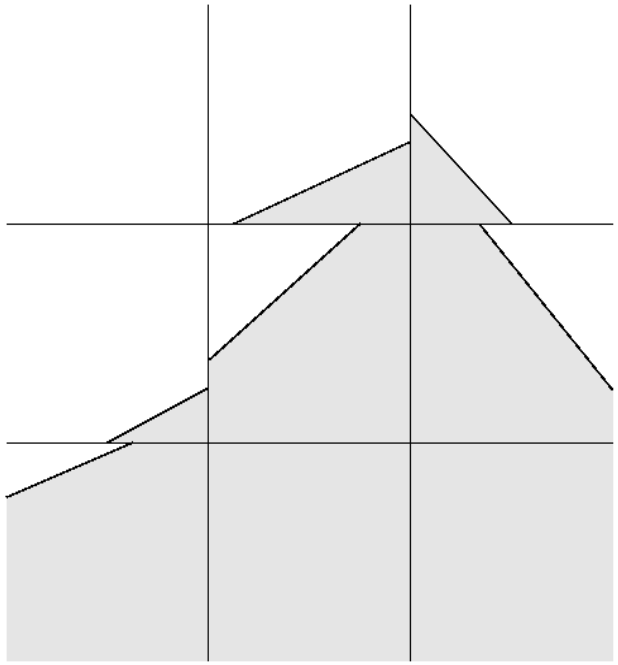




Multimaterial Arbitrary Lagrangian-Eulerian Methods

- Explicit Lagrangian phase (solves Lagrangian equations) – grid moves with the fluid
- Rezone phase – mesh moved (to improve geometric quality, smoothing, improve resolution)
- Remap phase – data transfer from Lagrangian grid to rezoned grid

- Material interface may not coincide with cell faces
- Multimaterial cells will then be introduced which contain more than one material



Multimaterial Lagrangian Hydro-Closure Models

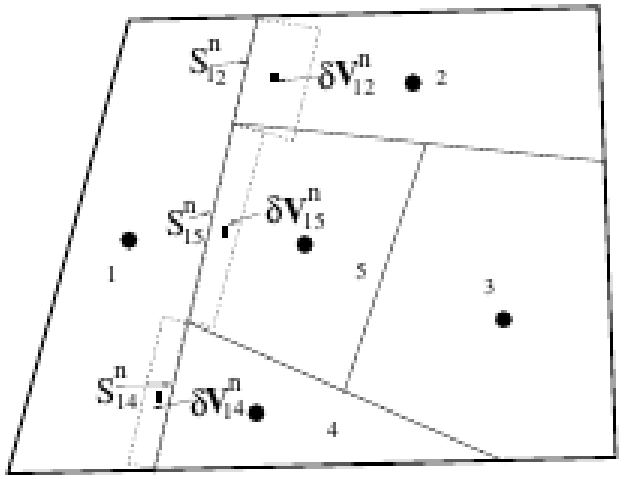
- Staggered grid – single velocity per node – separate velocities not available for different materials
- Each material component has its own volume fraction and set of state variables such as density, internal energy, pressure etc
- A single force acts on each node from each single or multimaterial cell must be determined to solve the momentum equation

Closure models for multimaterial cells are required to

- Advance the volume fractions (density) and internal energies for each material component during the Lagrangian step
- Define the force acting on each node in multimaterial cells

Types of Closure Model

- **Pressure Equilibrium**
  (Pressure Relaxation)
  - Enforced explicitly every time step e.g. Tipton's model (LLNL)
  - Does not require information about the interface geometry
- **Sub-Cell Dynamics**
  - Models pair wise interaction between materials
  - Requires interface geometry



Interface Aware Sub-Scale Dynamics (IA-SSD)

- IA-SSD is a sub-cell dynamics model
- Consists of two steps a bulk phase and a sub-cell dynamics step
- The bulk phase applies equal volumetric strain or an equal compressibility model and the sub-cell dynamics step introduces pair wise material interactions, which attempt to correct the solution obtained from the bulk phase
- Both steps are implemented within a predictor corrector time discretization scheme

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1) A. Barlow, R. Hill and M. Shashkov, Constrained optimization framework for Interface–aware sub-scale dynamics closure models for multimaterial cells in Lagrangian and arbitrary Lagrangian-Eulerian hydrodynamics, Journal of Computational Physics, 276 (2014) 92-135

Bulk phase (equal volumetric strain model)

- The state variable in the multimaterial cells are evolved by distributing the total cell volume change to the material components in proportion to the volume fractions. The internal energy can then be determine by

$$\varepsilon_{i,k}^{\,n+1} = \varepsilon_{i,k}^{\,n} + \Delta t \left(\frac{p_{i,k}^{\,n+\frac{1}{2}} + q^{n}}{M^{e}} \right) f_{i,k} \Delta . \bar{u}$$

- A volume fraction weighted average pressure is used to calculate the forces required to solve the momentum equation
- This ensures consistency between the energy and momentum equations for multimaterial cells
- **Multiphase artificial viscosity is required for voids.**

Sub-cell dynamics step

- A modified acoustic Riemann solver can be used to define the normal interface velocity v* and the interface pressure p*

$$v^* = \frac{p_2 - p_1}{\rho_1 c_1 + \rho_2 c_2} \qquad p^* = \frac{\rho_1 c_1 p_2 + \rho_2 c_2 p_1}{\rho_1 c_1 + \rho_2 c_2} + \bar{q}^*$$

$$\bar{q}^* = \frac{\rho_1 c_1 \rho_2 c_2 A \nabla . u}{\rho_1 c_1 + \rho_2 c_2}$$

where p_i is pressure, ρ_i is density, c_i sound speed of material component i, A is cell area and u are nodal velocities

- q* is like a linear artificial viscosity which is on in expansion and compression where $\nabla.u$ is calculated from the nodal velocities
- **For multimaterial cells containing a void material set p* to pressure in non-void material with a modified q***

Maximum volume and energy fluxes

- V* and p* are then used to define the maximum volume and internal energy flux's that can be exchanged between the material pairs
- If these are simply applied naively as they stand this can produce negative densities and internal energies, and pressure overshoots which will lead to a lack of robustness
- Robustness can however be obtained by applying a limiter function $0 \leq \psi \leq 1$ to the volume and energy flux's across each interface
- The value of this limiter function is chosen to ensure certain constraints on the; volumes, internal energies and pressures are satisfied for all material components

Total volume change

- The volume change of each material component is then given by a combination the volume change from the bulk and the limited sub-scale dynamics fluxes

$$\Delta V_{i,k} = f_{i,k}\Delta V_i + \sum_j \chi_j \Delta v_j$$

- The bulk update can be viewed as a low order solution and a combination of bulk plus unlimited subscale dynamics as the high order. The limiter function will then move the solution towards the low order as required to satisfy the constraints
- The full unlimited fluxes are calculated for each interface material pair.
- Limiter values are the determined for more than two materials by either solving a quadratic optimization problem with linear constraints as in [1] or by solving a series of two material cases for which there is an explicit solution with partial updates in between each pair

Limiter value for Volume constraint

- To ensure the volume of the materials either side of an interface does not become too small define volume flux limit

$$dV\lim_{i,k} = (k_{bot} - 1.0)\, f_{i,k} V_i$$

where $k_{bot} \sim 0.5$

- If $dV_{i,k} < dV\lim_{i,k}$ then

$$\psi v_{i,k} = \frac{dV\lim_{i,k}}{dV_{i,k}}$$

- Else

$$\psi v_{i,k} = 1$$

- **K_{bot}= 0.0 for void materials to allow voids to close completely**

Limiter value for Internal energy constraint

- To avoid the Internal energy of either material component going negative:

$$dE\lim_{i,k} = -m_{i,k}\varepsilon_{i,k}$$

- If $dE_{i,k} < dE\lim_{i,k}$ then

$$\psi\varepsilon_{i,k} = \frac{dE\lim_{i,k}}{dE_{i,k}}$$

- Else

$$\psi\varepsilon_{i,k}=1$$

- **$\psi\varepsilon_{i,k}=1$ for void materials**

Limiter value for Pressure constraint 1

- Limits Pressure of either material component from getting too close to the average cell pressure
- Pressure at end of bulk phase estimated from isentropic approximation:

$$Pb_{i,k}^{n+1} = p_{i,k}^{n} - \frac{\rho_{i,k}^{n}(c_{i,k}^{2} + \frac{2q_{i,k}^{n}}{\rho_{i,k}^{n}})dV_i^{n}}{V_i^{n}}$$

- Volume fraction weighted average used as average cell pressure

$$Pb_i^{n+1} = \sum_k f_{i,k}^{n} Pb_{i,k}^{n+1}$$

- **Pb_i = 0.0 if void material one of pair of materials for interface**

Limiter value for Pressure constraint 2

- The volume change to approach average pressure is now given by

$$dVtp_{i,k}^{n+1} = \frac{k_t f_{i,k}^n V_i^n (Pb_{i,k}^n - Pb_i^n)}{\rho_{i,k}^n (c_{i,k}^2 + \frac{2q_{i,k}^n}{\rho_{i,k}^n})}$$

where k_t~0.99

- The pressure limiter then depends on whether the bulk pressure is above or below the target pressure

Limiter value for Pressure constraint 3

If $Pb_{i,k} > Pb_i$ then

If $dV_{i,k}=0$ then

$\psi p_{i,k}=1.0$

else if $dV_{i,k}<0$ then

$\psi p_{i,k}=0.0$

else if $|dV_{i,k}| > |dVtp_{i,k}|$ then

$$\psi p_{i,k} = \frac{|dVtp\lim_{i,k}|}{|dV_{i,k}|}$$

If $Pb_{i,k} < Pb_i$ then

If $dV_{i,k}=0$ then

$\psi p_{i,k}=1.0$

else if $dV_{i,k}>0$ then

$\psi p_{i,k}=0.0$

else if $|dV_{i,k}| > |dVtp_{i,k}|$ then

$$\psi p_{i,k} = \frac{|dVtp\lim_{i,k}|}{|dV_{i,k}|}$$

- **$\psi p_{i,k}=1.0$ for void materials**

Limiter values for two material case

- A single limiter value is required for each material interface
- For the two material problem this is obtained directly from the minimum of the six limiter values for the three constraints in two materials

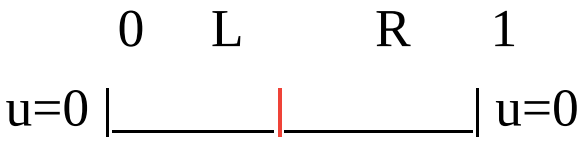
$$\psi = \min(\psi\nu_1, \psi\nu_2, \psi\varepsilon_1, \psi\varepsilon_2, \psi p_1, \psi p_2)$$

Limiter values for n material case

- In [1] the constrained optimization problem is solved using third party software. A simpler approach is taken here which builds on the explicit solution for the 2 materials to satisfy the constraints
- The new approach solves the 2 material case at each interface in turn, applies the limited volume and energy fluxes across the interface and then performs an intermediate update of the volume fractions, densities and internal energies
- The constraints are re-evaluated for the next interface using the partially updated quantities
- **The pressure limiting must be performed using a pressure average that only includes the two materials either side of the interface to avoid locking**
- The constraints are then satisfied once all the 2 material pairs have been updated

Sod shock tube problem

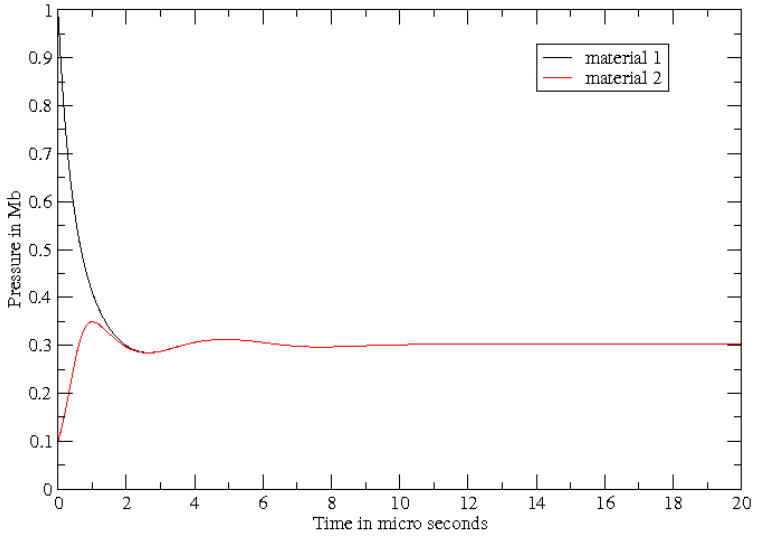
Statement of the problem

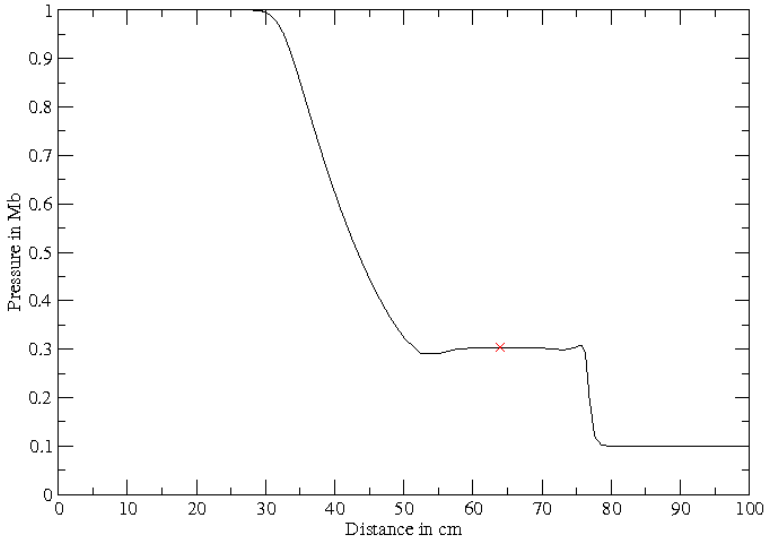


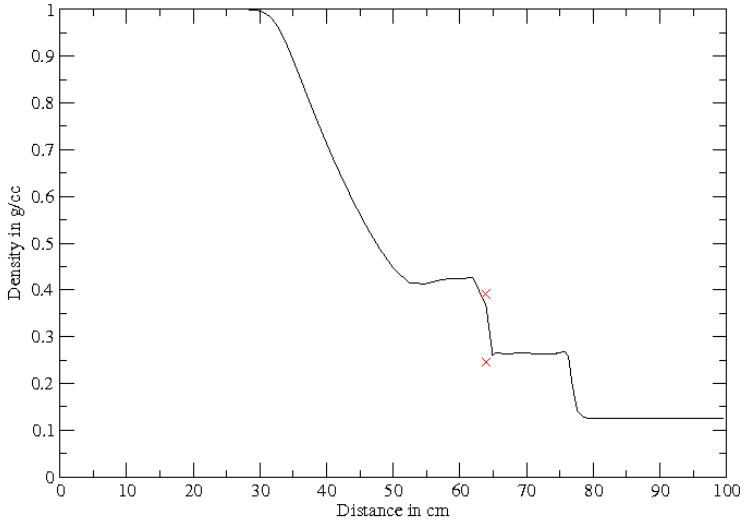
$p=(\gamma-1)\rho\varepsilon$	$p=(\gamma-1)\rho\varepsilon$
$\gamma=1.4$	$\gamma=1.4$
$p=1$	$p=0.1$
$\rho=1$	$\rho=0.125$
$u=0$	$u=0$

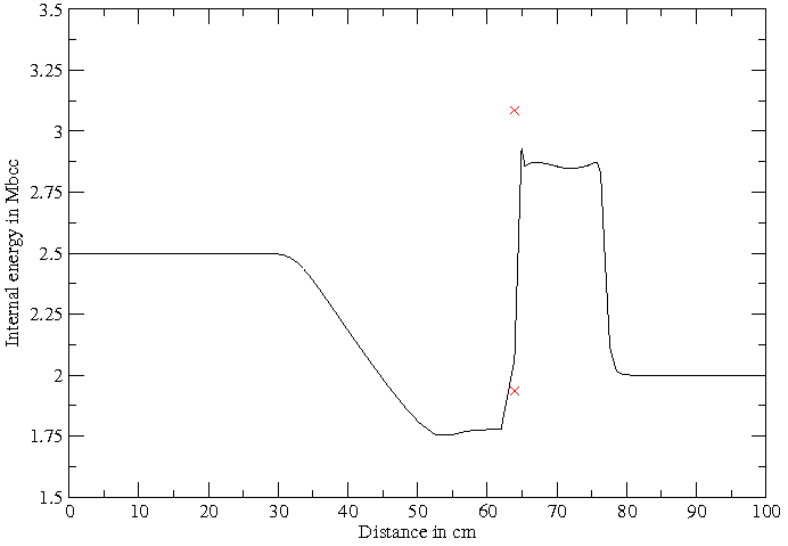
multimaterial cell
f=0.5

Sod with SSD closure model t=15.0 μs

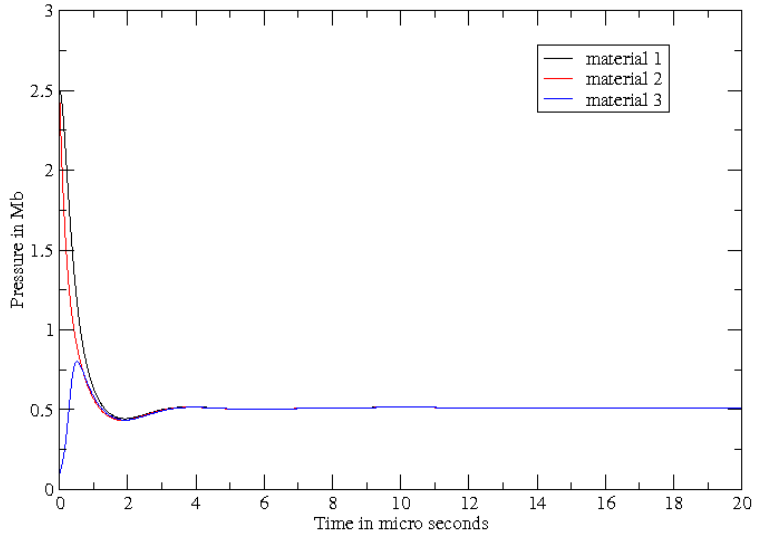


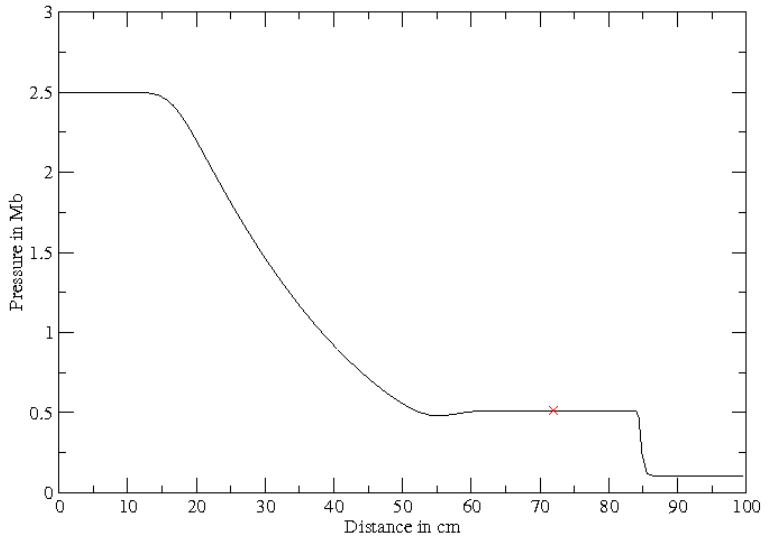


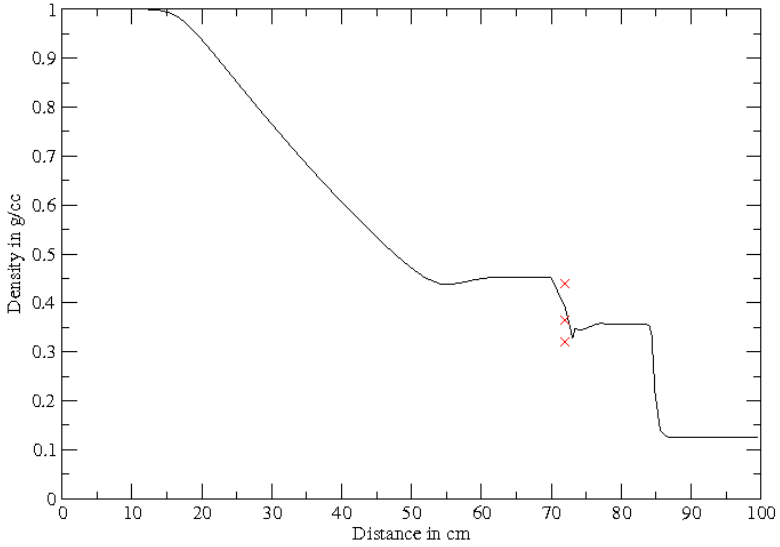


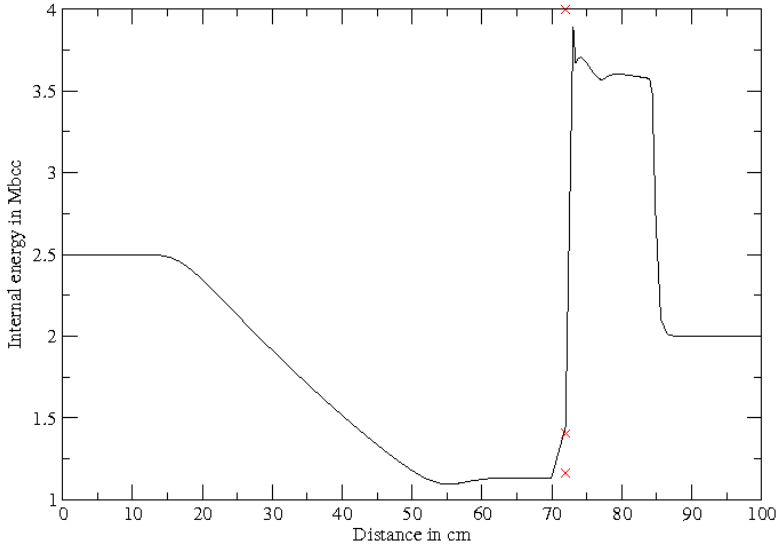


3 material modified Sod f=(1/3,1/3,1/3) H H L

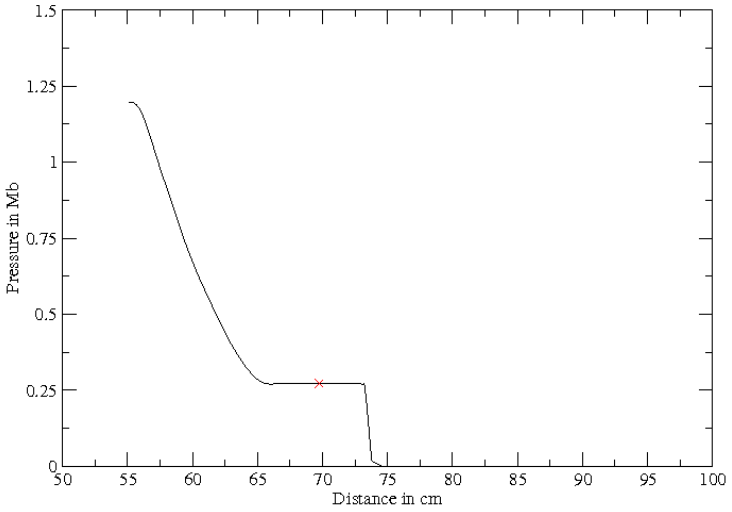


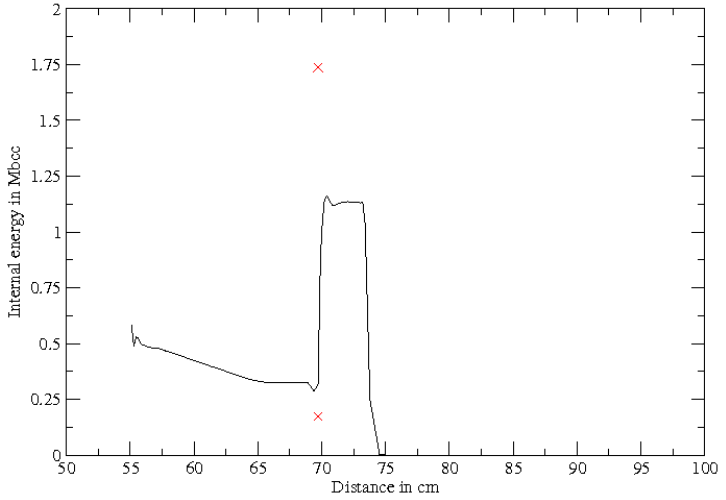




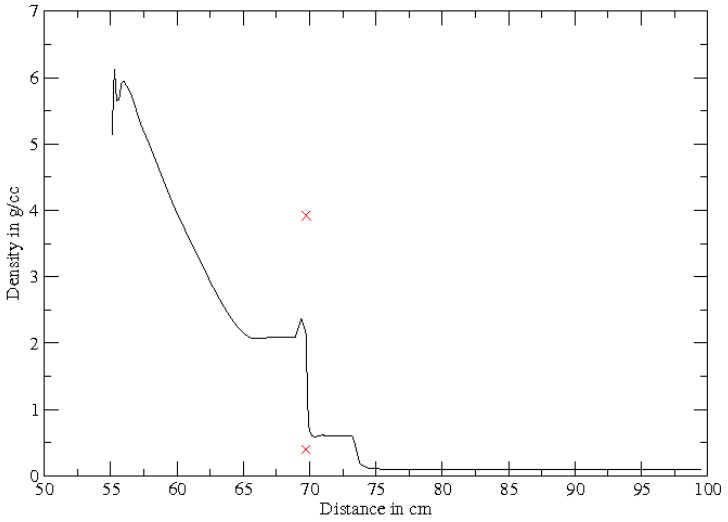


Piston problem with single phase q f=(0.5,0.5)

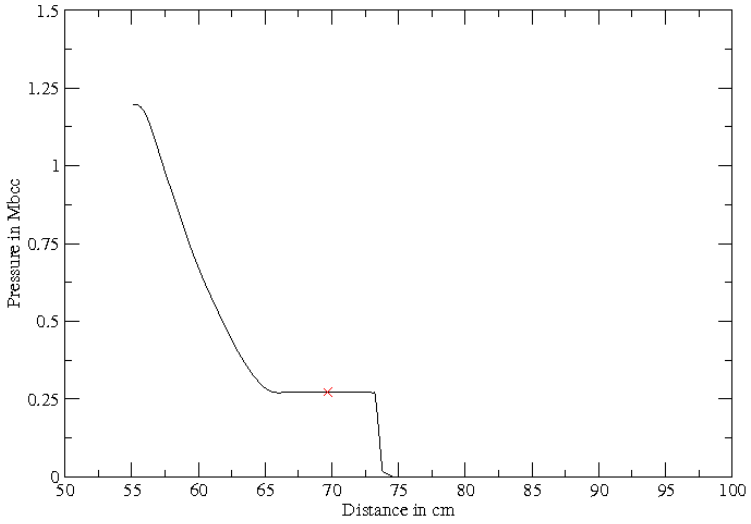


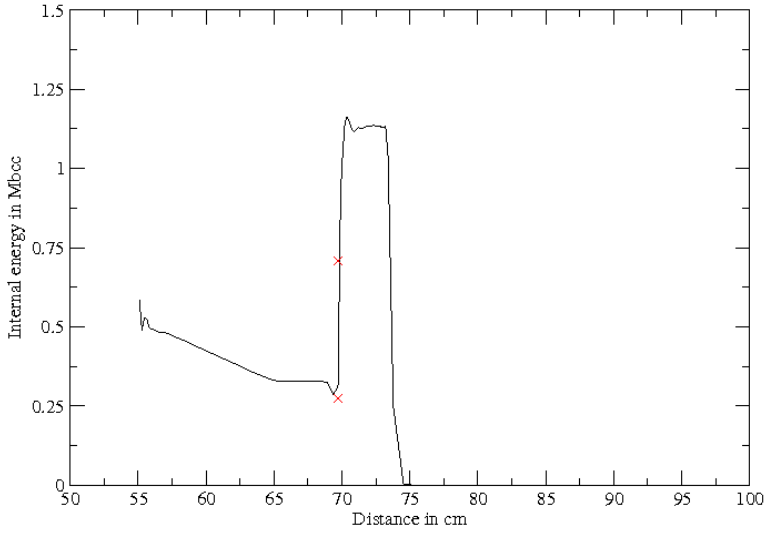


- Shock interaction with multimaterial cell
- Left boundary moving at 1 cm/μs to generate a shock which interacts with material interface
- Lagrangian mesh motion
- Initial multimaterial cell has f=(0.5,0.5)
- Two materials both cold internal energy e=0 Mbcc
- Left material ρ=1.0 g/cc and right material ρ=0.1 g/cc

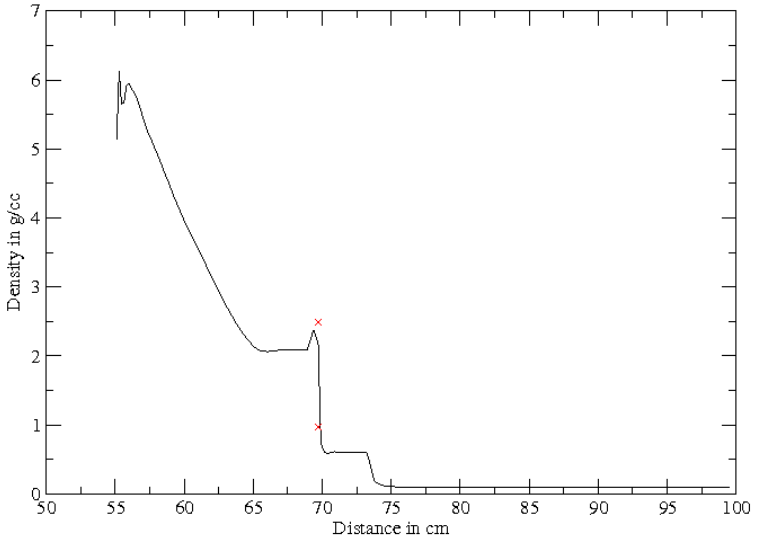


Piston problem with multi-phase q f=(0.5,0.5)



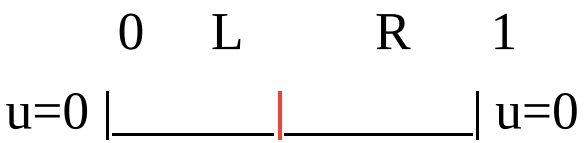


- The bulk phase can be improved significantly by introducing multi-phase artificial viscosities and sub-zonal pressures
- Separate q's and subzonal pressures calculated for each material component using component densities and sound speeds, but single phase values for velocities
- Volume fraction averaged values used to calculate corner forces used in momentum equation
- Corner forces also calculated for each material component and used to evolve component internal energies



Expansion into vacuum problem

Statement of the problem



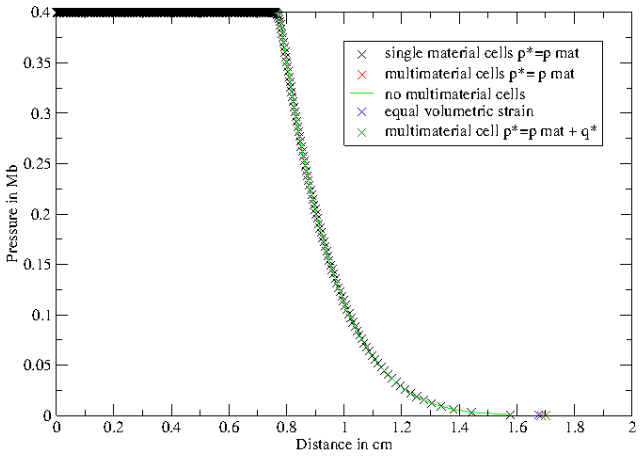
$p=(\gamma-1)\rho\varepsilon$ void

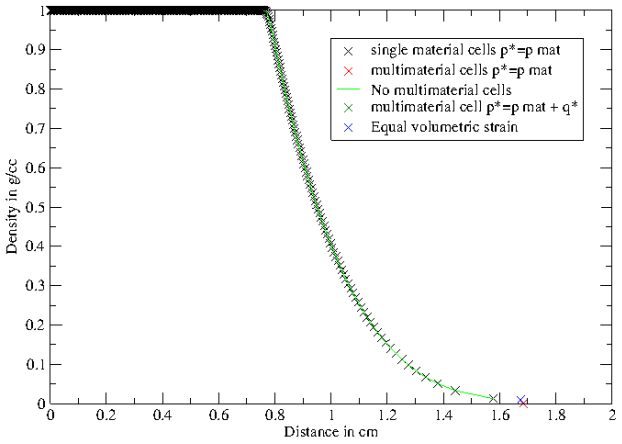
$\gamma=1.4$

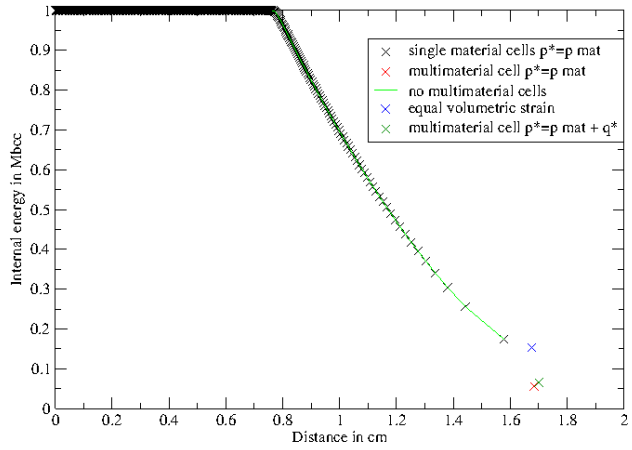
p=0.4	p=0.0
ρ=1	ρ=0.0
u=0	u=0

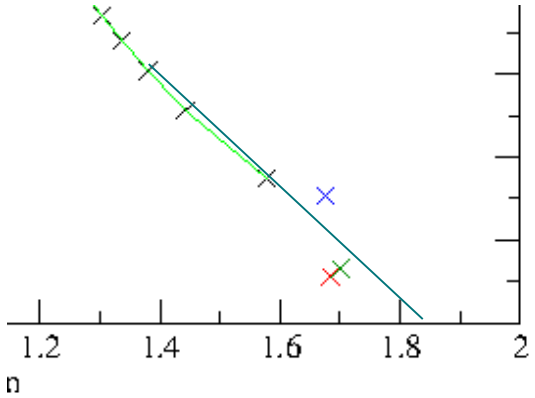
multimaterial cell
f=0.005

Expansion into vacuum with SSD t=0.35 μs

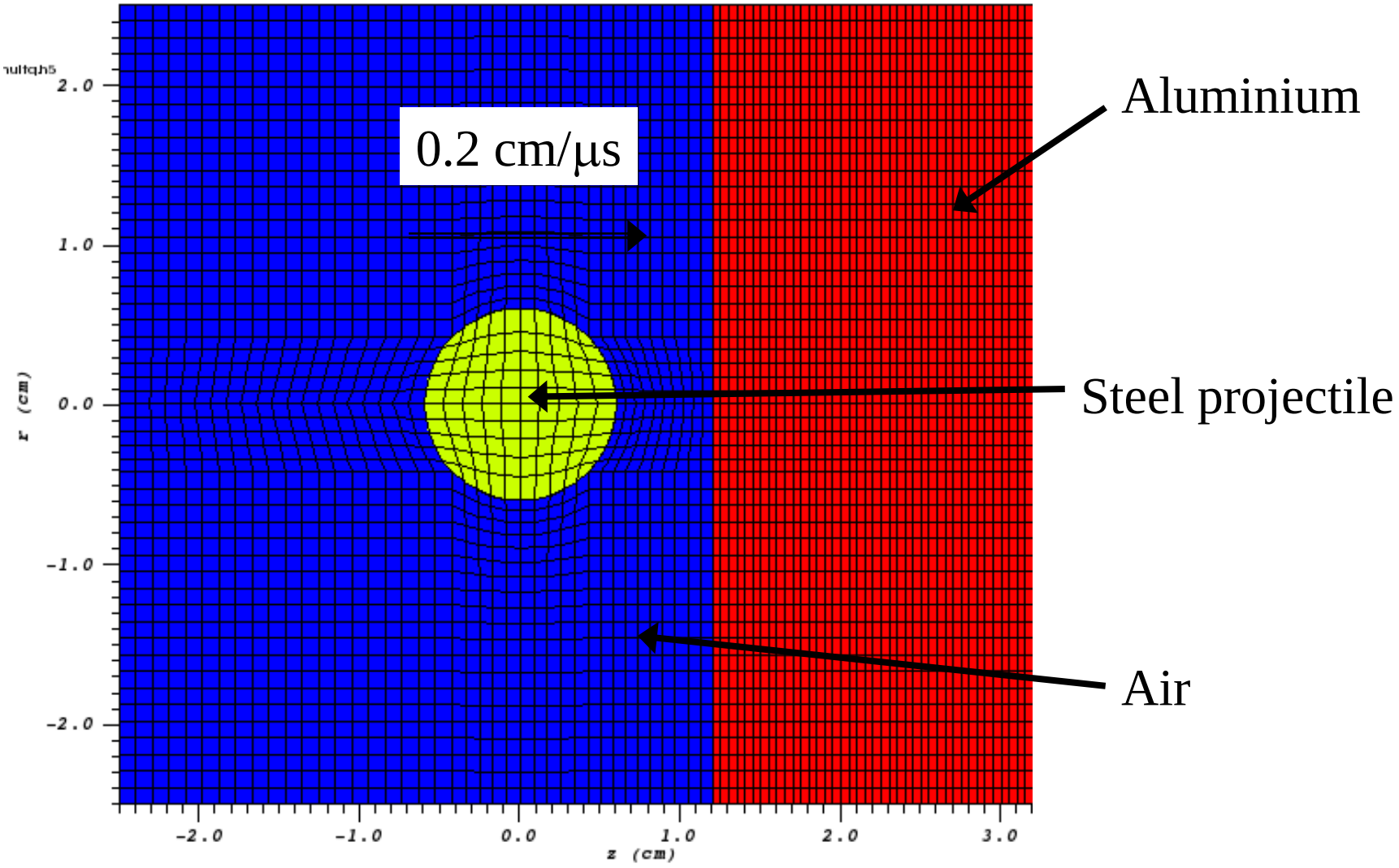




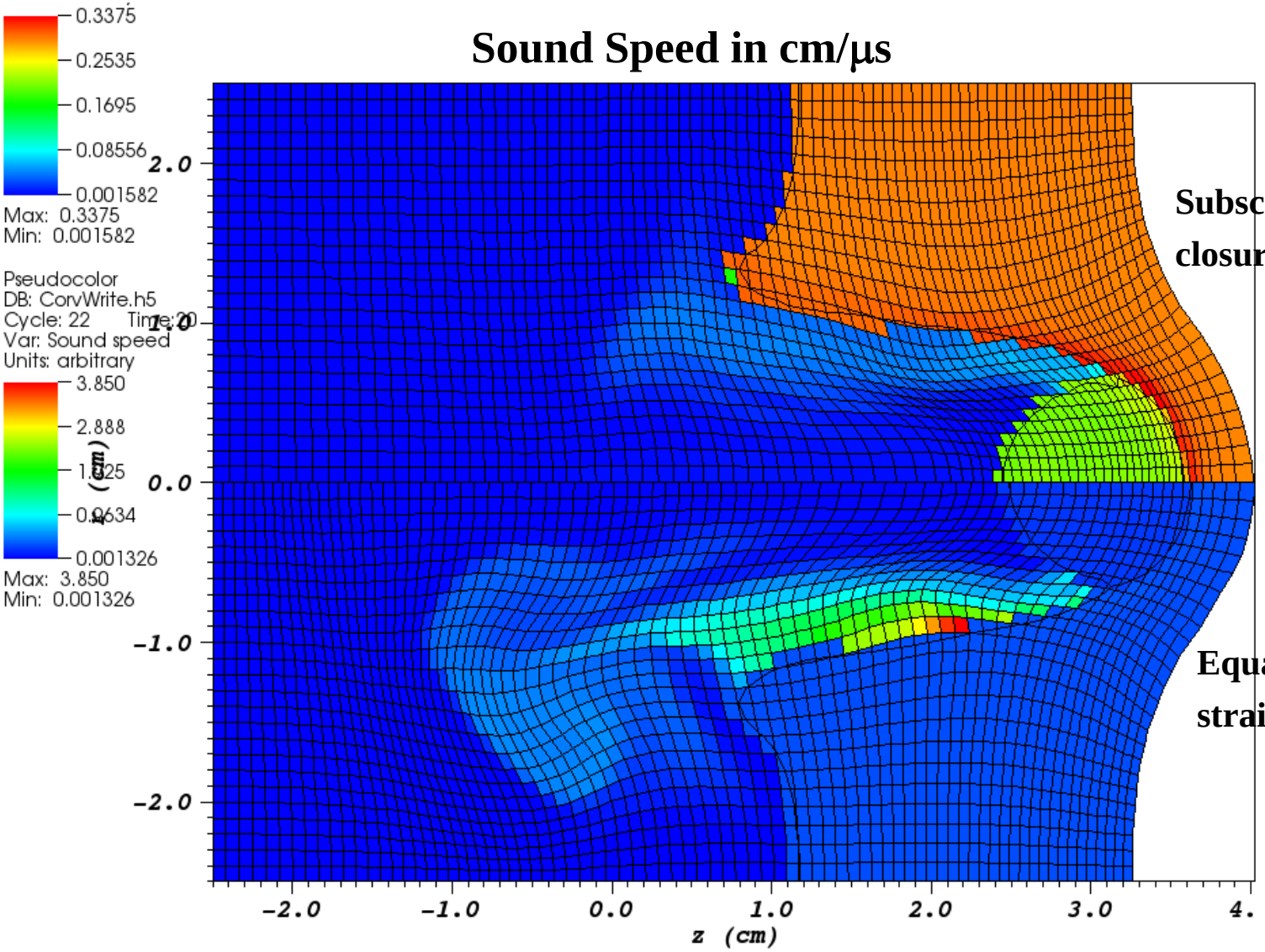




Projectile impact t=0.0 μs



Projectile impact t=20.0 μs



Conclusions

- Further improvements and simplifications have been made to the interface aware sub-scale-dynamics closure model [1]
- A simpler method has been developed for extending the interface aware subcell dynamics scheme to n materials
- The approximate Riemann solver has also been modified to introduce an artificial viscosity like term which avoids the need for construction of component velocities
- The importance of multiphase viscosities and subzonal pressures in the bulk phase has also been demonstrated and a simple method for their introduction described
- The method has also been extended to allow void closure and propagation through void

Future Work

- Extend closure model to include additional interface physics:
  - Void opening
  - Elastoplastic flow
  - Slide
  - Friction