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Title: Interface-aware sub-scale dynamics closure model

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Interface-aware sub-scale dynamics closure model

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Motivation

- Material interfaces may not coincide with the computational mesh
  - Arbitrary Lagrangian-Eulerian (ALE) schemes
- Multimaterial cells
  - Each material has its own mass (density), internal energy and pressure
  - Single velocity for the multimaterial nodes
  - Single pressure for the momentum update
  - The closure model is used to generate this pressure, and update material variables

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Closure Model Classes

- Pressure equilibrium/relaxation
  - Tipton’s pressure relaxation model Shashkov, Int. J. Num. Meth. Fluids, 2007
    - Expression for $p_i^{n+1/2}$ derived assuming the flow is isentropic
    - Relaxation term added resembling linear viscosity
    - Solve a system of linear equations for $p^{n+1/2}$ and $\delta V_i^{n+1/2}$, which has an explicit solution
    - Computed values are used in an internal energy update.
    - Material pressures found by individual equation of state calls
- Modelling sub-cell dynamics Barlow, ECCOMAS Computational Fluid Dynamics Conference, 2001
  - Interface-aware sub-scale dynamics (IASSD)
    - Knowledge of multimaterial cell topology is used to generate fluxes between neighbouring materials
    - Fluxes are optimised based upon limiting constraints for each of the material parameters

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IASSD Design Principles

- Preservation of contact
  - If all materials in the multimaterial cell have the same initial pressure, they should not change
- Pressure equilibrium
  - After some time, the material pressures should equilibrate
- Conservation of total energy

IASSD Model Overview

- Each material has its own mass, internal energy and pressure
- Material volumes are determined by associated volume fractions
- The multimaterial cell topology is determined from the Moment of Fluid (MoF) interface reconstruction algorithm. Ahn, Shashkov, J. Comput. Phys., 2007
- Material properties are updated via:
  - a bulk update, arising from the overall movement of the cell
  - sub-scale fluxes, arising from material interactions
- Sub-scale fluxes are optimised based upon conditions imposed on the material properties

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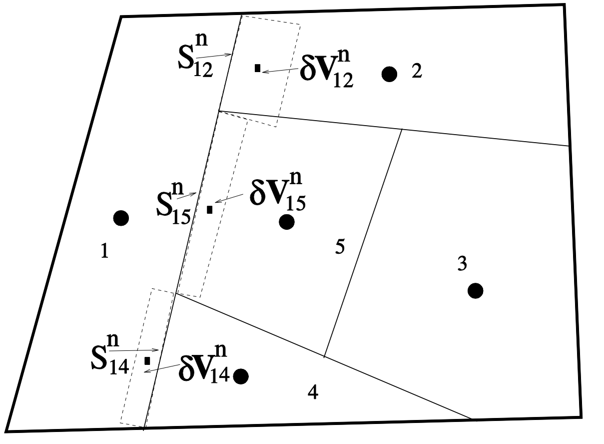
IASSD – Cell Topology

- The MoF interface reconstruction method provides a subset of pure polygons and an updated centroid for each material

- The intersection of the pure polygons provides:
  - the length of the interface, $S_{i,k}$, between materials i and k.
  - The set of materials neighbouring each material, $\mathcal{M}(i)$. E.g. $\mathcal{M}(1) = \{2,4,5\}, \mathcal{M}(4) = \{1,3,5\}$

- Maximum volume exchanges are estimated from an acoustic Riemann solver

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



IASSD – Positivity of Material Volume

- The material volumes update is given by

$$V_i^{n+1} = \underbrace{V_i^n + f_i^n \Delta V^{n+1}}_{= V_i^{f,n+1}} + \underbrace{\sum_{k \in \mathcal{M}(i)} \Psi_{i,k} \delta V_{i,k}^{\max}}$$

bulk update — sub-scale fluxes

- With the necessary condition

$$0 < V_i^{n+1} < V^{n+1}$$

because mass cannot disappear during the Lagrangian calculation.

- In order to optimise the sub-scale fluxes, the volume constraint is chosen as

$$\alpha_{bot} f_i^n V^{n+1} \leq V_i^{n+1}$$

with $0 < \alpha_{bot} \leq 1$.

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IASSD – Positivity of Material Volume

- The limiter Ψ is desired to be as close to the 'higher order' solution ($\Psi = 1$) as possible in the range $0 \le \Psi \le 1$.

- We need to ensure there is at least one choice of Ψ that will always satisfy the volume update.

- Setting all $\Psi_{i,k} = 0$:

$$\overbrace{\alpha_{bot}}^{>0}\overbrace{f_i^n}^{>0}\overbrace{V^{n+1}}^{>0} \le \overbrace{V_i^{n+1}}^{=f_i^n V^{n+1}} \qquad \Rightarrow \qquad 0 < V_i^{n+1}.$$

Also, because

$$\sum_i V_i^{n+1} = V^{n+1},$$

for an arbitrary i_0, we have

$$V_{i_0}^{n+1} = V^{n+1} - \sum_{i \neq i_0} \overbrace{V_i^{n+1}}^{>0} \qquad \Rightarrow \qquad V_{i_0}^{n+1} < V^{n+1}$$

$$\Rightarrow \qquad V_i^{n+1} < V^{n+1}$$

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IASSD – Positivity of Internal Energy

- The internal energy update is given by

$$\varepsilon_i^{n+1} = \underbrace{\varepsilon_i^n - \frac{p_i^n f_i^n}{m_i}\Delta V^{n+1}}_{=\,\varepsilon_i^{f,n+1}} - \frac{1}{m_i}\sum_{k\in\mathcal{M}(i)} p_{i,k}^{*}\Psi_{i,k}\delta V_{i,k}^{\max}$$

where

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

with $\kappa = \rho c$.

- Internal energy must be positive, so the optimisation condition on the sub-scale fluxes is

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

IASSD – Positivity of Internal Energy

- Again, with the limiter in the range $0 \leq \Psi \leq 1$, we need to ensure that there is at least one solution satisfying the positivity constraint.

- Setting all $\Psi_{i,k} = 0$: $m_i \varepsilon_i^n - p_i^n f_i^n \Delta V^{n+1} > 0$

- Where the internal energy update in this form is assumed to be positive with the following constraint on Δt :

  - Cell under compression ($\Delta V^{n+1} < 0$) : $\underbrace{m_i \varepsilon_i^n}_{>0} \underbrace{- p_i^n f_i^n \Delta V^{n+1}}_{>0} > 0$ $\Rightarrow$ No additional constraint on Δt.
  - Cell under expansion ($\Delta V^{n+1} > 0$) : $m_i \varepsilon_i^n < p_i^n f_i^n \Delta V^{n+1}$

or $\Delta V^{n+1} < \frac{m_i \varepsilon_i^n}{p_i^n f_i^n}$, and with $m_i = \rho_i^n V_i^n = \rho_i^n f_i^n V^n$

$p_i^n = (\gamma_i - 1) \rho_i^n \varepsilon_i^n$

$\frac{\Delta V^{n+1}}{V^n} < \frac{1}{\gamma_i - 1}$ which is a constraint on Δt because $\text{DIV}\, \mathbf{u} = \frac{\mathbf{1}}{\boldsymbol{V}} \frac{\boldsymbol{dV}}{\boldsymbol{dt}}$ $\Rightarrow$ $\Delta \text{t} < \frac{1}{(\gamma_i - 1)\text{DIV}\, \mathbf{u}}$

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IASSD – Pressure Equilibrium

- The material pressure update is given as

$$p_i^{n+1} = \underbrace{p_i^n - \frac{\rho_i^n (c_i^n)^2}{V_i^n} f_i^n \Delta V^{n+1}}_{= p_i^{f,n+1}} - \frac{\rho_i^n (c_i^n)^2}{V_i^n} \sum_{k \in \mathcal{M}(i)} \Psi_{i,k} \delta V_{i,k}^{\max}$$

- To achieve pressure equilibrium we choose that material pressures will relax to (at least not diverge from) an average cell pressure.

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

- If $p_i^{f,n+1} \geq \bar{p}$ then we require $\alpha_i \bar{p} + (1 - \alpha_i) p_i^{f,n+1} \leq p_i^{n+1} \leq p_i^{f,n+1}$

- If $p_i^{f,n+1} \leq \bar{p}$ then we require $p_i^{f,n+1} \leq p_i^{n+1} \leq \alpha_i \bar{p} + (1 - \alpha_i) p_i^{f,n+1}$

where $0 < \alpha_i < 1$ is a parameter to control the rate of equilibration.

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IASSD – Pressure Equilibrium

- Ensuring there is a solution to the pressure constraints with $0 \leq \Psi \leq 1$, we test the case that all $\Psi_{i,k} = 0$.

- If $p_i^{f,n+1} \geq \bar{p}$ then

$$\alpha_i \bar{p} + (1 - \alpha_i) p_i^{f,n+1} \leq p_i^{f,n+1} \leq p_i^{f,n+1}$$

$$\alpha_i \bar{p} + (1 - \alpha_i) p_i^{f,n+1} - p_i^{f,n+1} \leq \quad 0 \quad \leq 0$$

$$\underbrace{\alpha_i}_{>0} \underbrace{\left(\bar{p} - p_i^{f,n+1}\right)}_{<0} \leq \quad 0 \quad \leq 0$$

- If $p_i^{f,n+1} \leq \bar{p}$ then

$$p_i^{f,n+1} \leq p_i^{f,n+1} \leq \alpha_i \bar{p} + (1 - \alpha_i) p_i^{f,n+1}$$

$$0 \leq \quad 0 \quad \leq \alpha_i \bar{p} + (1 - \alpha_i) p_i^{f,n+1} - p_i^{f,n+1}$$

$$0 \leq \quad 0 \quad \leq \underbrace{\alpha_i}_{>0} \underbrace{\left(\bar{p} - p_i^{f,n+1}\right)}_{>0}$$

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IASSD – Limiting Sub-Scale Fluxes

- A quadratic optimisation scheme with linear constraints is employed to achieve a global solution with all $\Psi_{i,k}$ as close to unity as possible.
- The optimisation problem is formulated as

Schittkowski. QL: A Fortran Code for Convex Quadratic Programming

$$\text{maximise} \quad \sum_{i}^{n_{mat}} \sum_{k \in \mathcal{M}(i)} \Psi_{i,k}^2$$

subject to

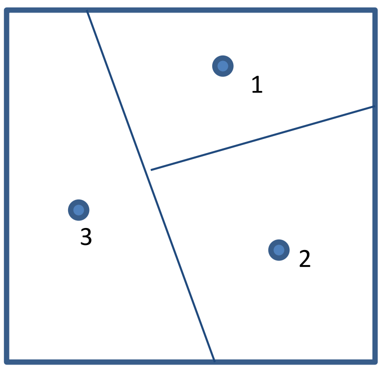
$$\sum_{k \in \mathcal{M}(i)} \Psi_{i,k} F_{i,k}^{\delta\varepsilon} \leq m_i \varepsilon_i^{f,n+1}$$

$$\begin{cases} 0 \leq \sum_{k \in \mathcal{M}(i)} \Psi_{i,k} F_{i,k}^{\delta V} \leq \dfrac{\alpha_i V_i^n}{\rho_i^n \left(c_i^n\right)^2} \left(p_i^{f,n+1} - \bar{p}\right) & \text{if} \quad p_i^{f,n+1} > \bar{p} \\ \max\left[(\alpha_{bot} - 1) V_i^{f,n+1}, \dfrac{\alpha_i V_i^n}{\rho_i^n \left(c_i^n\right)^2} \left(p_i^{f,n+1} - \bar{p}\right)\right] \leq \sum_{k \in \mathcal{M}(i)} \Psi_{i,k} F_{i,k}^{\delta V} \leq 0 & \text{if} \quad p_i^{f,n+1} < \bar{p} \end{cases}$$

IASSD – Limiting Sub-Scale Fluxes

Three Material Example

$p_1^{f,n+1} > p_2^{f,n+1} > \bar{p} > p_3^{f,n+1}$



- The optimisation problem for this multimaterial cell is

maximise

$$\Psi_{1,2}^2 + \Psi_{1,3}^2 + \Psi_{2,3}^2$$

subject to

$$F_{1,2}^{\delta\varepsilon}\Psi_{1,2} + F_{1,3}^{\delta\varepsilon}\Psi_{1,3} \le m_1 \varepsilon_1^{f,n+1}$$
$$-F_{1,2}^{\delta\varepsilon}\Psi_{1,2} + F_{2,3}^{\delta\varepsilon}\Psi_{2,3} \le m_2 \varepsilon_2^{f,n+1}$$
$$-F_{1,3}^{\delta\varepsilon}\Psi_{1,3} - F_{2,3}^{\delta\varepsilon}\Psi_{2,3} \le m_3 \varepsilon_3^{f,n+1}$$

$$\Psi_{i,k} = \Psi_{k,i} \quad F_{i,k}^{\delta V} = -F_{k,i}^{\delta V} \quad F_{i,k}^{\delta\varepsilon} = -F_{k,i}^{\delta\varepsilon}$$

$$F_{i,k}^{\delta V} = \delta V_{i,k}^{\max} \quad F_{i,k}^{\delta\varepsilon} = p_{i,k}^{*}\delta V_{i,k}^{\max}$$

$$0 \le F_{1,2}^{\delta V}\Psi_{1,2} + F_{1,3}^{\delta V}\Psi_{1,3} \le \frac{\alpha_1 V_1^n}{\rho_1^n (c_1^n)^2}\left(p_1^{f,n+1} - \bar{p}\right)$$

$$0 \le -F_{1,2}^{\delta V}\Psi_{1,2} + F_{2,3}^{\delta V}\Psi_{2,3} \le \frac{\alpha_2 V_2^n}{\rho_2^n (c_2^n)^2}\left(p_2^{f,n+1} - \bar{p}\right)$$

$$\max\left[(\alpha_{bot} - 1)V_3^{f,n+1}, \frac{\alpha_3 V_3^n}{\rho_3^n (c_3^n)^2}\left(p_3^{f,n+1} - \bar{p}\right)\right] \le -F_{1,3}^{\delta V}\Psi_{1,3} - F_{2,3}^{\delta V}\Psi_{2,3} \le 0$$

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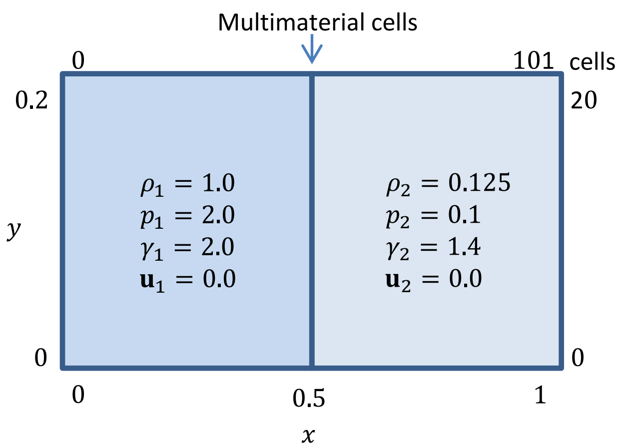
Modified Shock Tube

Initial Conditions

- The modified shock tube is repeated for progressively stronger shocks
- The IASSD and Tipton closure models are benchmarked against pure cell simulations



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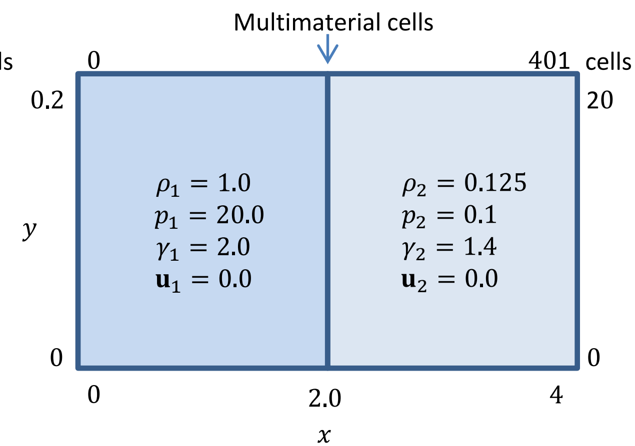

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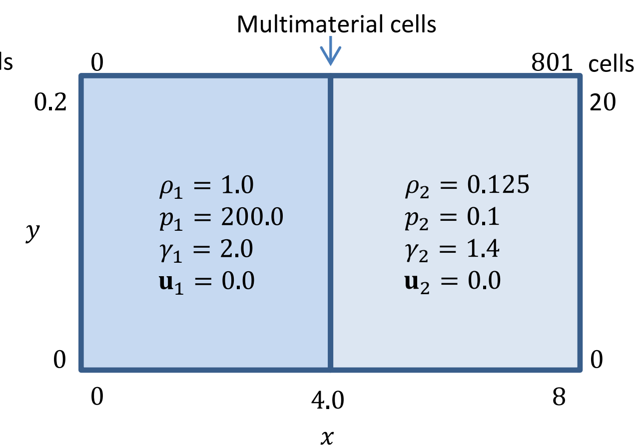

Case 3

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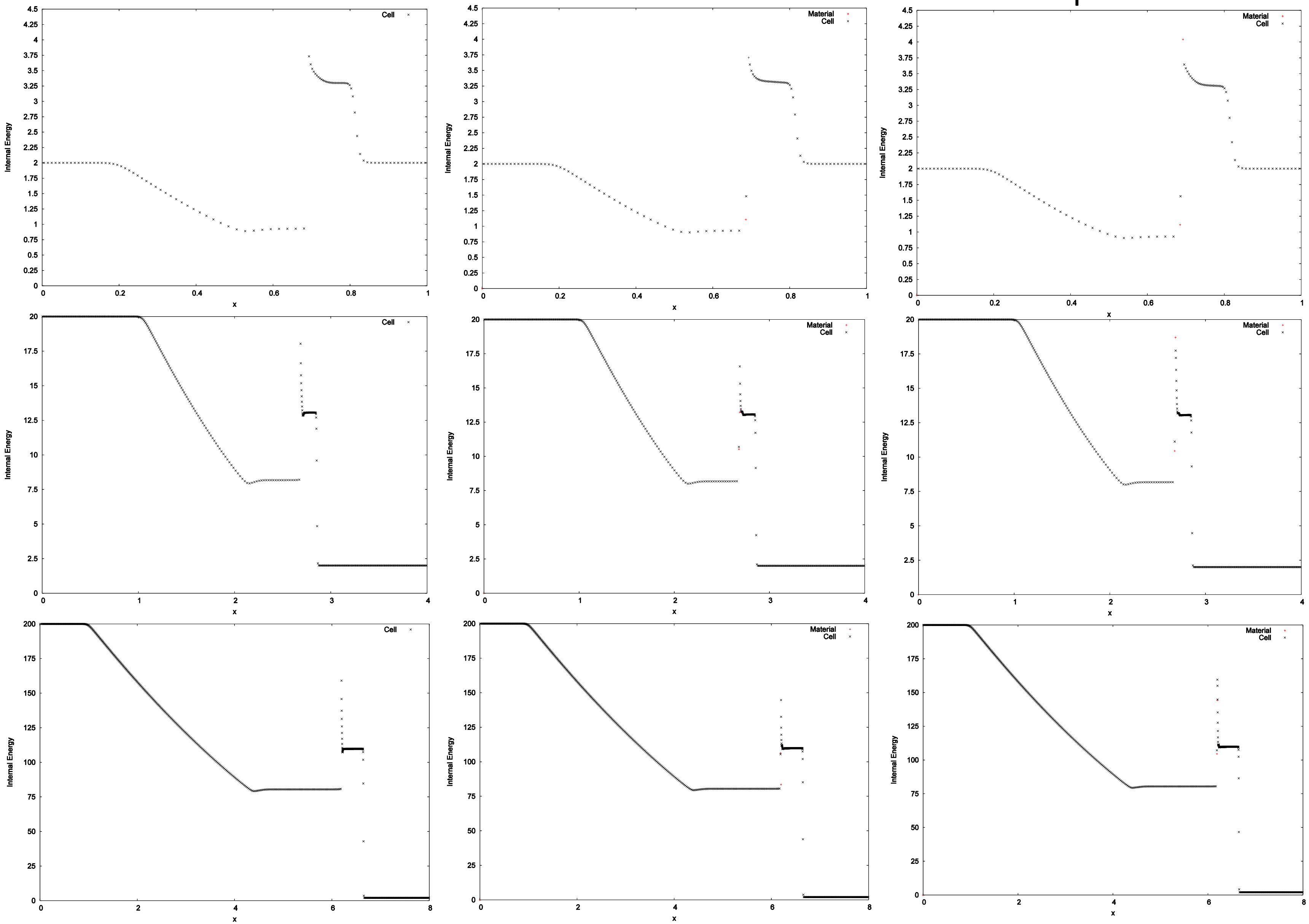
Modified Shock Tube

Internal Energy Profiles

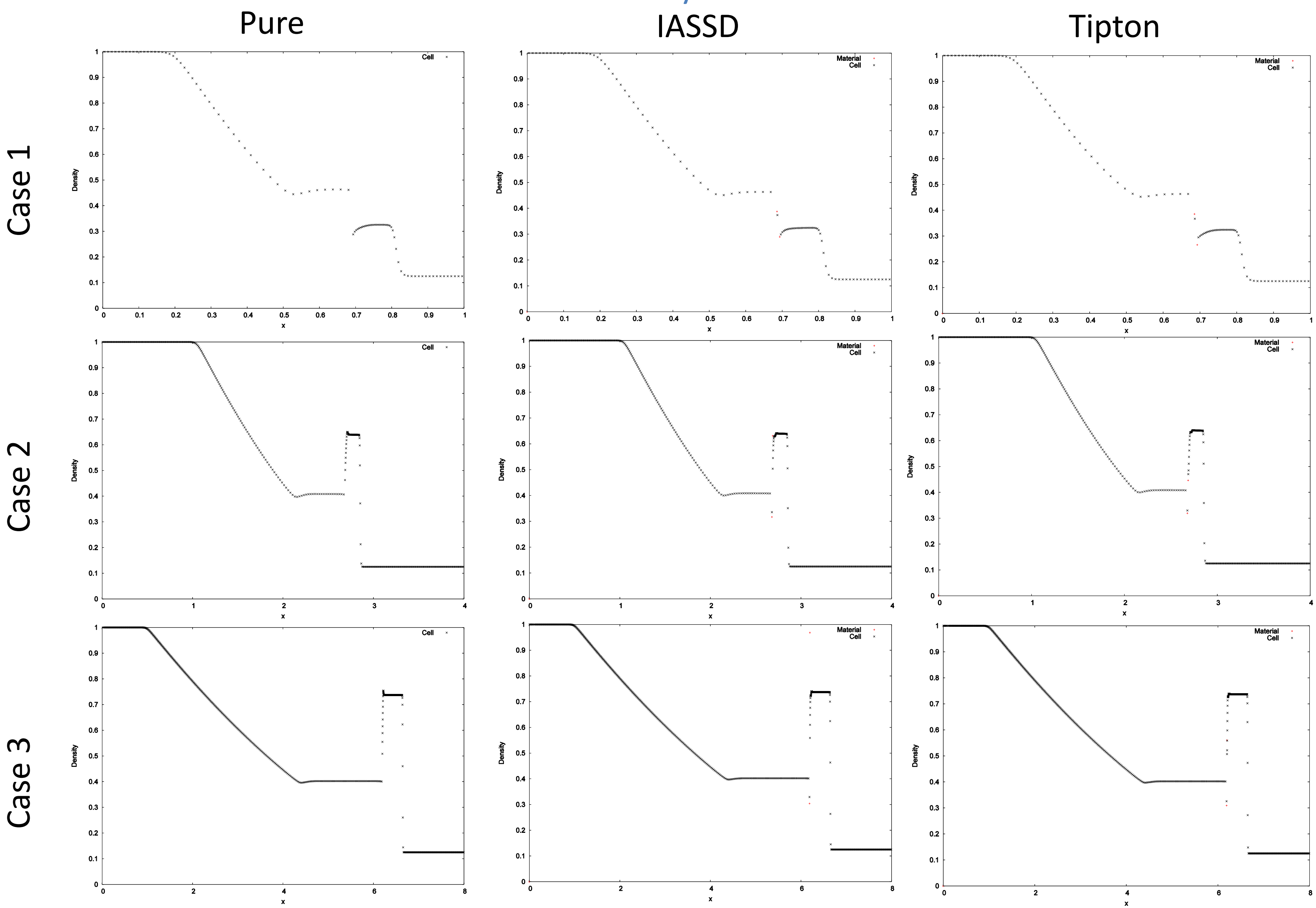
Pure | IASSD | Tipton

Case 1 | Case 2 | Case 3



Modified Shock Tube

Density Profiles

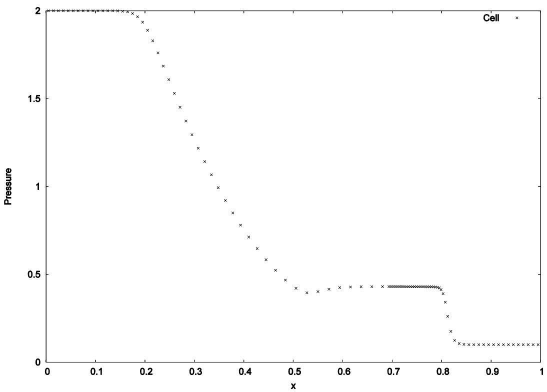


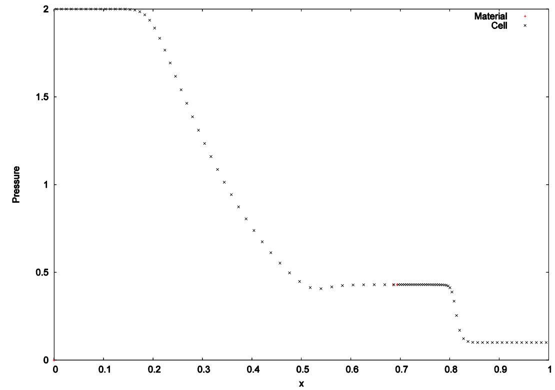
Modified Shock Tube

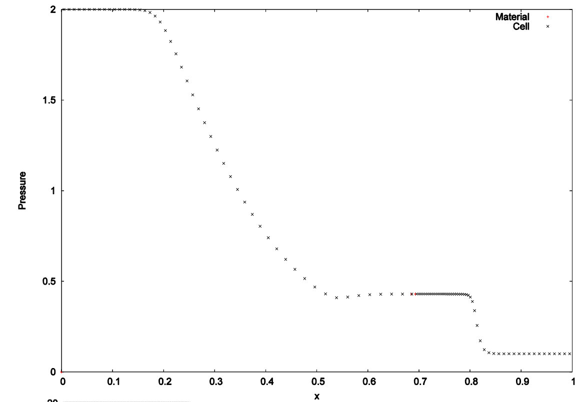
Pressure Profiles

Pure | IASSD | Tipton

Case 1







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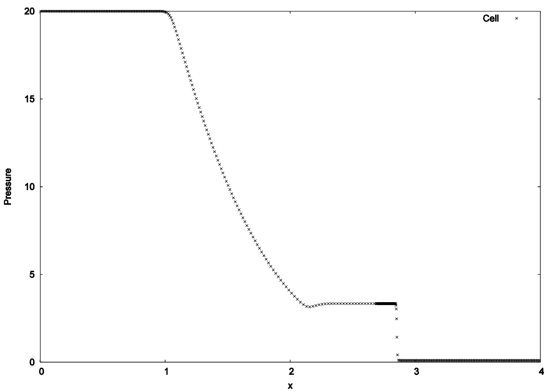

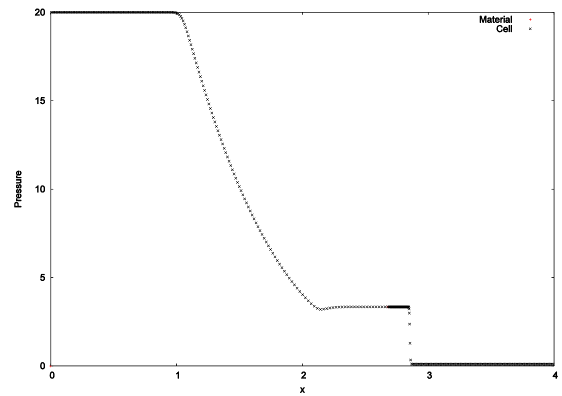

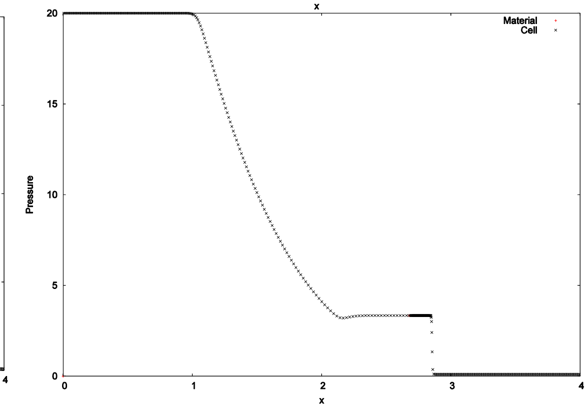

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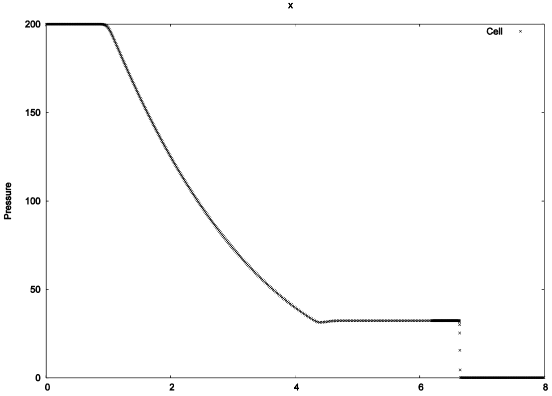
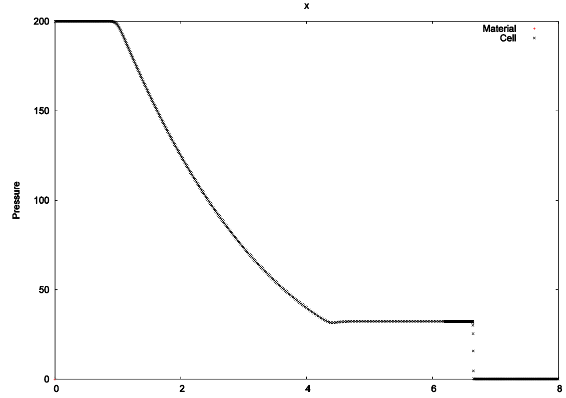
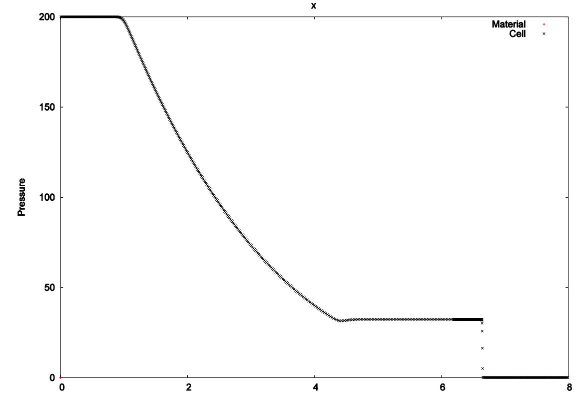






Modified Shock Tube

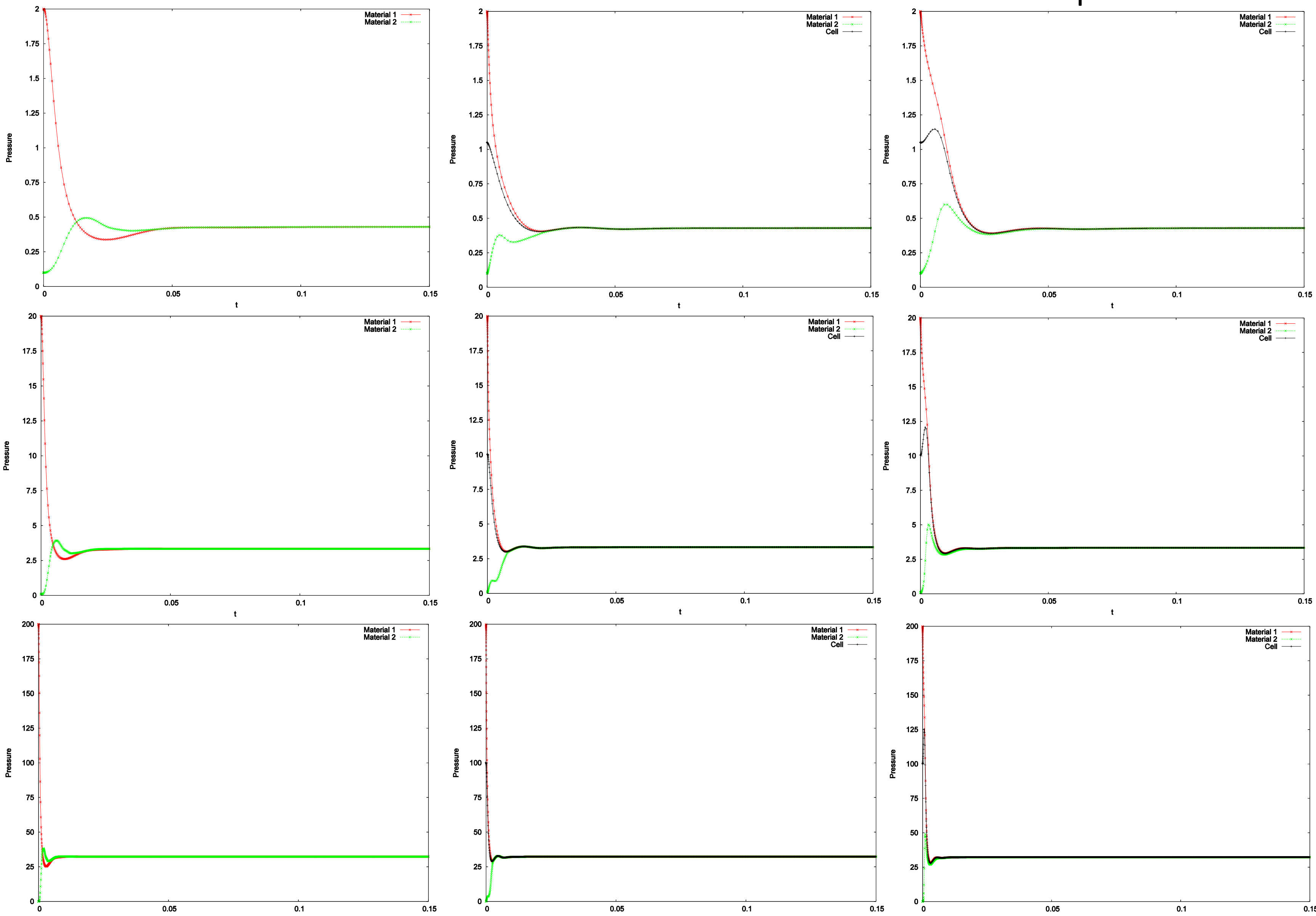
Pressure Equilibrium

Pure | IASSD | Tipton

Case 1

Case 2

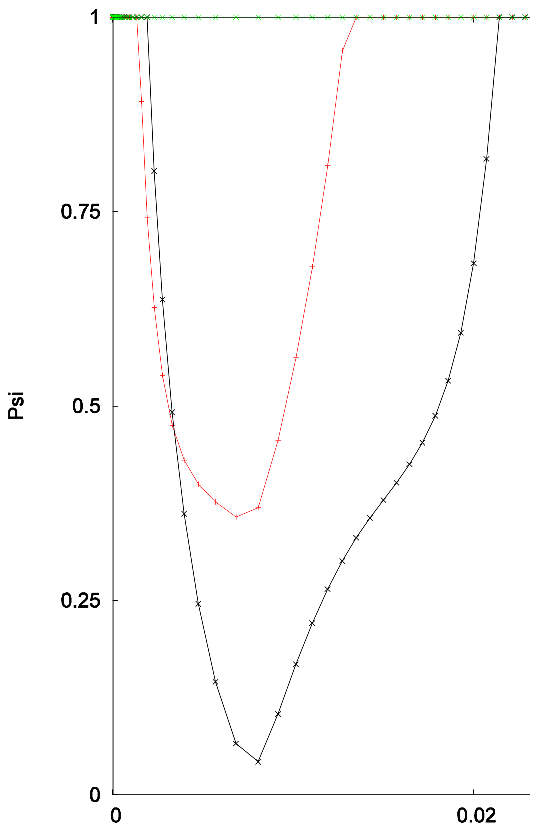
Case 3



Modified Shock Tube

Limiter Evolution

Case 1



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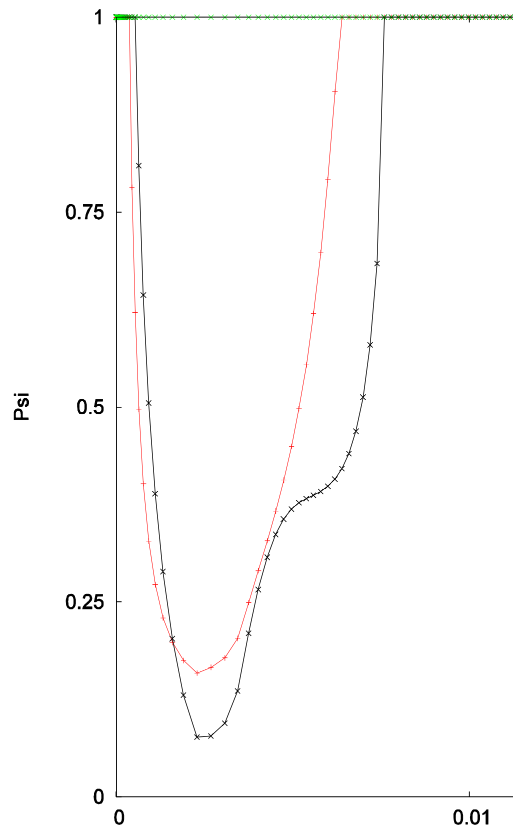

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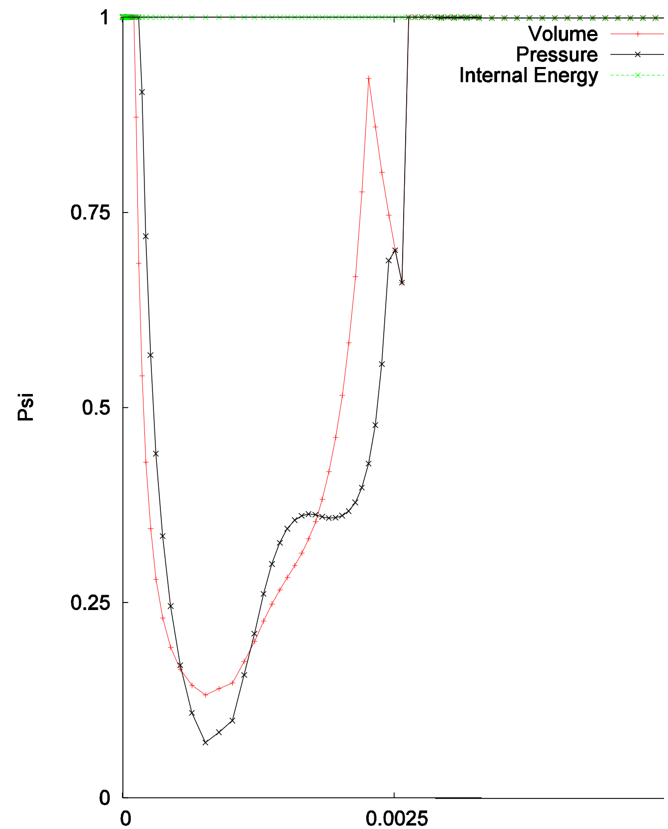
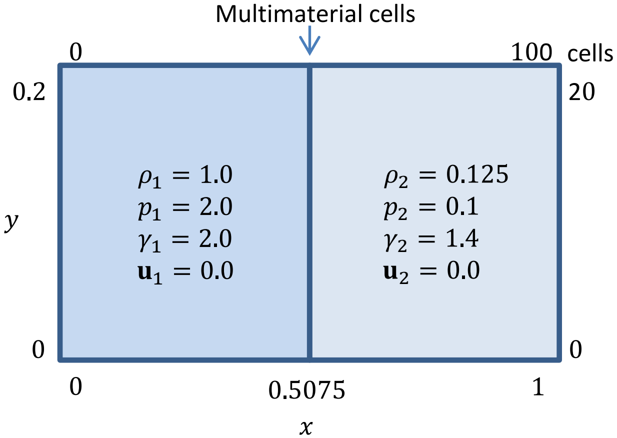


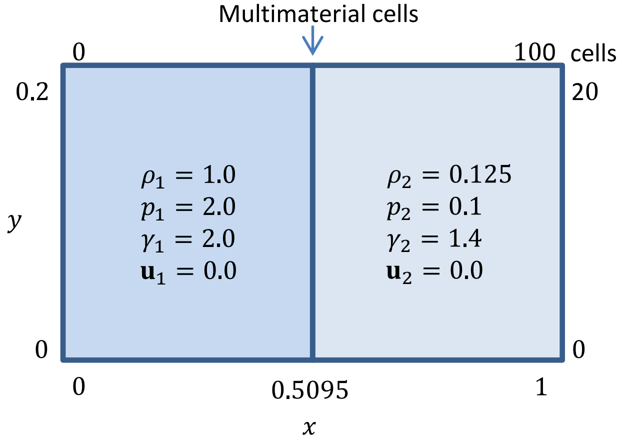
Small Volume Fraction Shock Tube

Initial Conditions

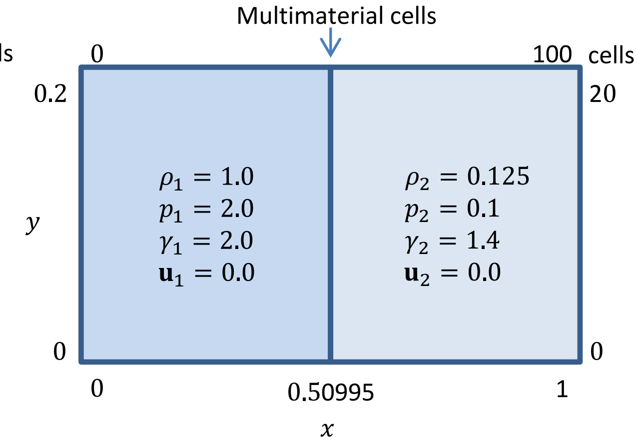
- The modified shock tube is repeated with progressively smaller volume fractions
- The IASSD and Tipton closure models are benchmarked against pure cell simulations



Case 1



Case 2



Case 3

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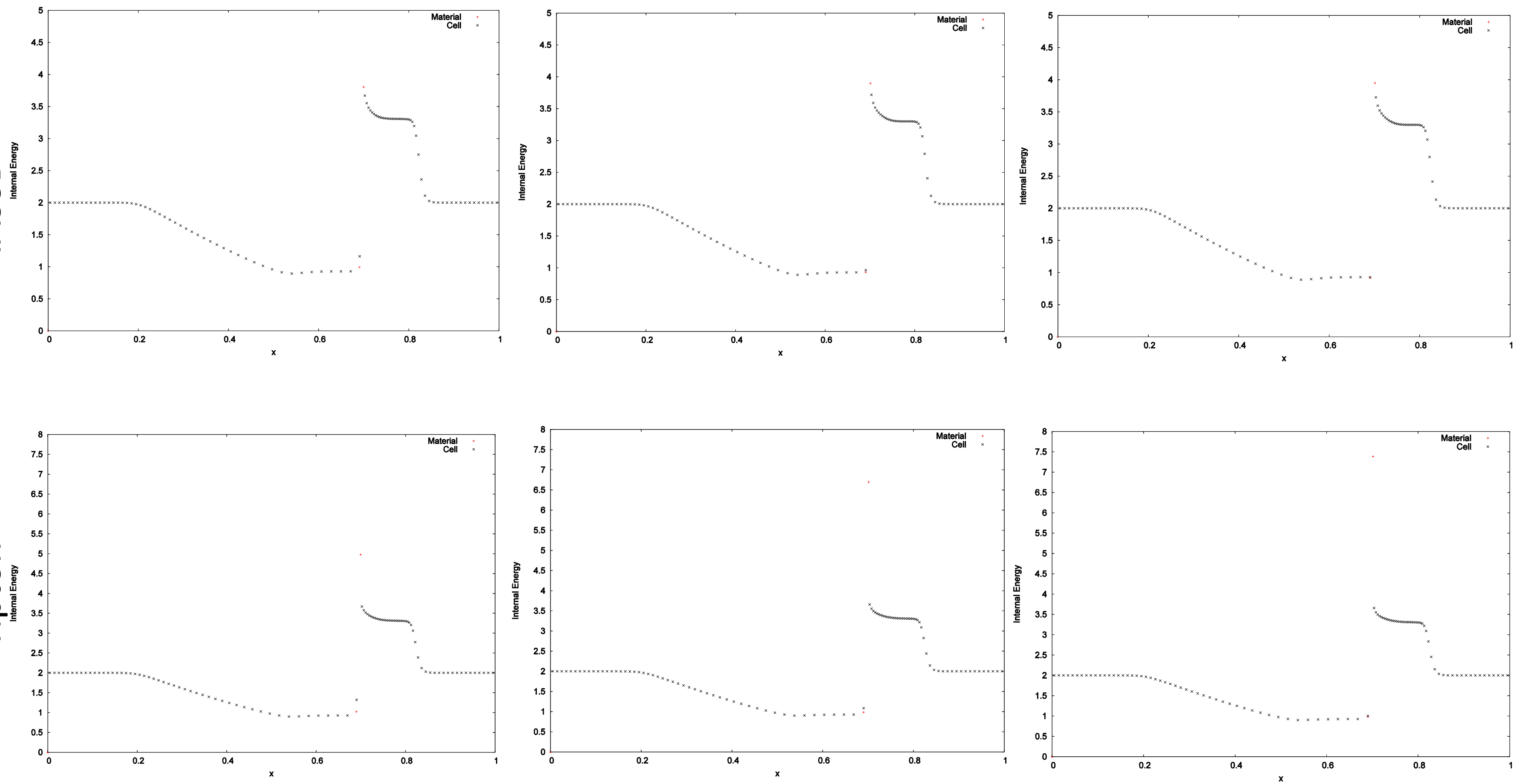
Small Volume Fraction Shock Tube

Internal Energy Profiles

Case 1 | Case 2 | Case 3

IASSD

Tipton



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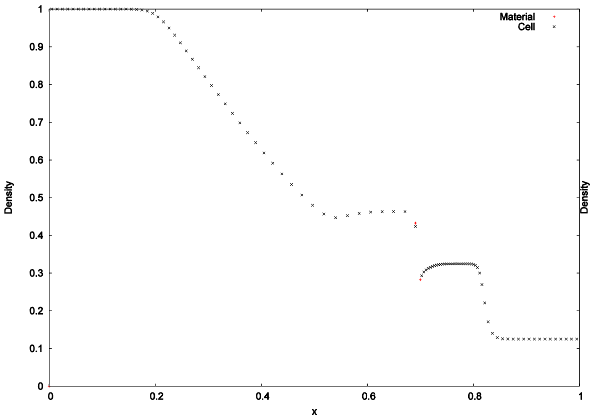
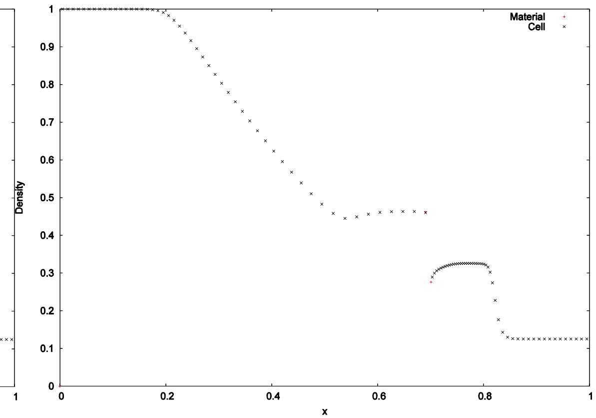
Small Volume Fraction Shock Tube

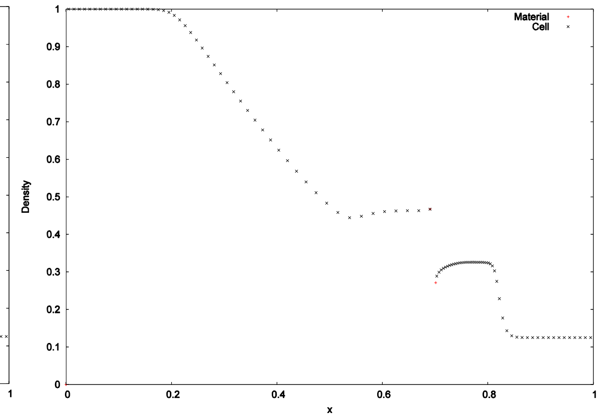
Density Profiles

Case 1 | Case 2 | Case 3

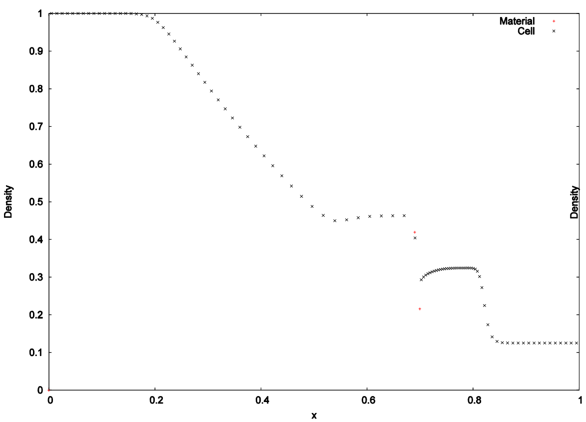
IASSD

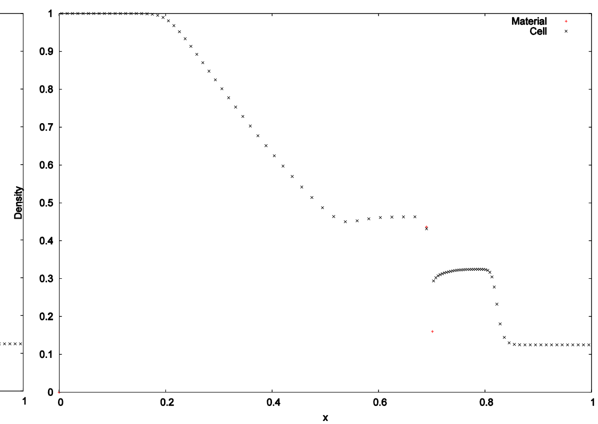


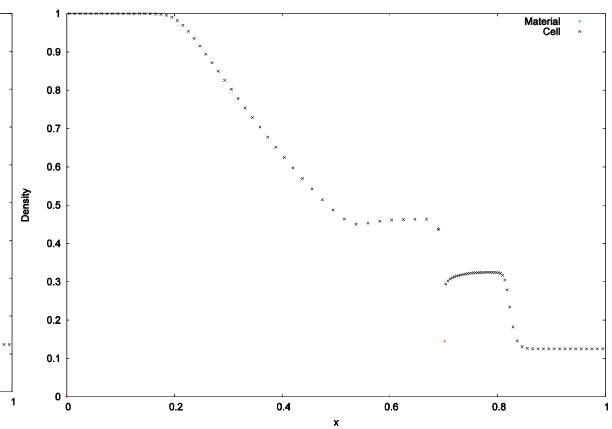




Tipton







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Small Volume Fraction Shock Tube

Pressure Equilibrium

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IASSD

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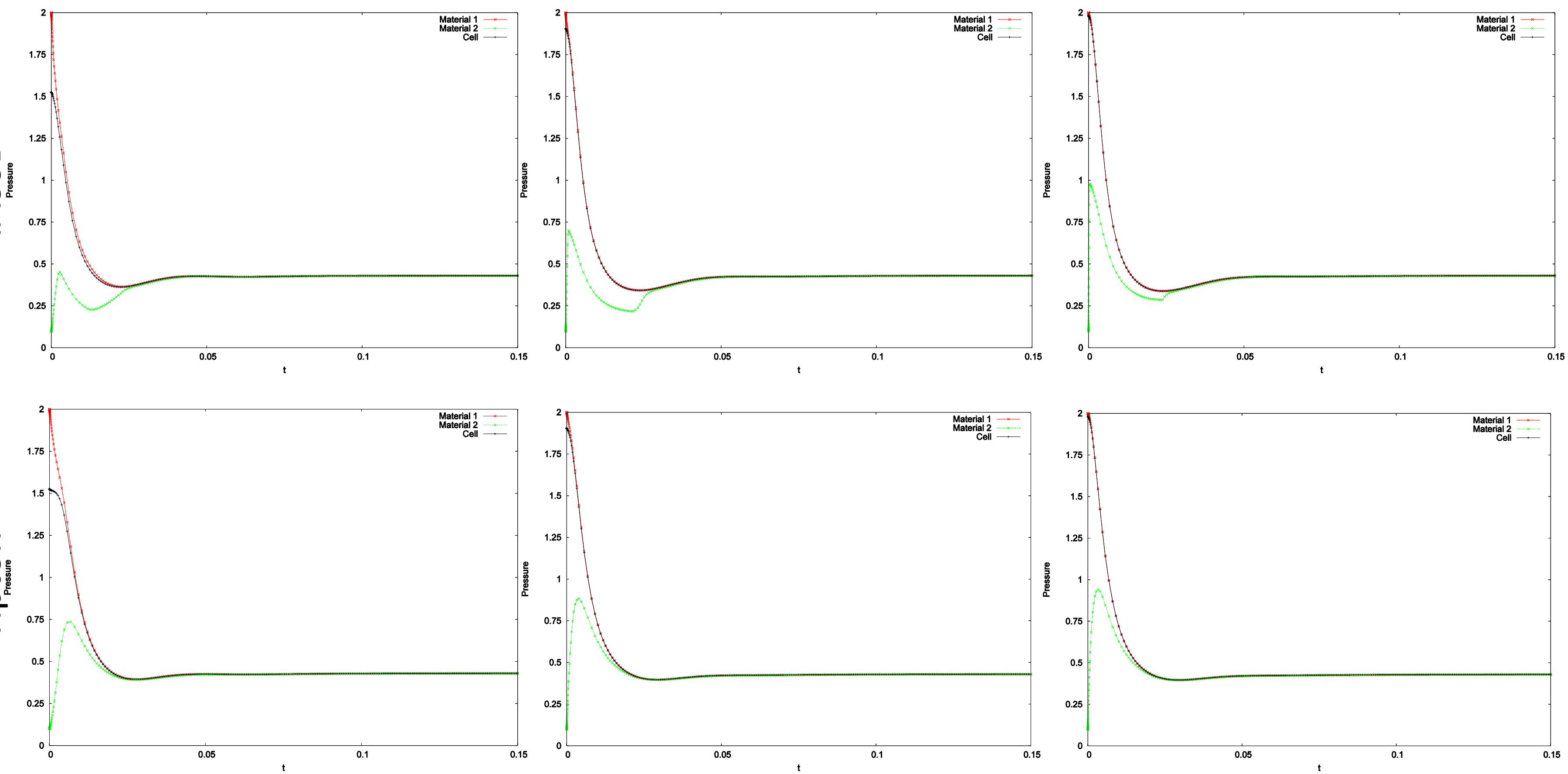

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Conclusions

- IASSD material parameters give a good match to the values in pure neighbouring cells
- IASSD behaviour appears less dependent upon the size of the shock or volume fractions.

Future Work

- Investigate role of parameters
- Multidimensional
- Multimaterial (more than two materials)
- ALE

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- K. Schittkowski. QL: A Fortran Code for Convex Quadratic Programming – User's Guide, February 2011, available at http://www.klaus-schittowski.de

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