

Multi-Material Closure Models for 1-D Lagrangian Hydrodynamics

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Overview

- **Lagrangian hydrodynamics of two materials in 1-D**
 - Two material, one-velocity model leads to a closure problem.
- **Three different staggered-mesh discretizations**
 - The approaches used in computations are presented.
- **Several different closure models**
 - All use pressure relaxation in the mixed cell as a physically-motivated assumption.
- **Comparison of computational results**
 - Pressure equilibration behavior for two test problems
- **Conclusions**



Two-material Lagrangian hydrodynamics in 1-D presents several open issues.

- Conservation laws govern the flow of inviscid, non-heat-conducting, compressible fluids in the Lagrangian frame:

$$\text{Mass:} \quad \rho^0 \frac{D\tau}{Dt} - \frac{\partial u}{\partial x} = 0$$

$$\text{Momentum:} \quad \rho^0 \frac{Du}{Dt} + \frac{\partial P}{\partial x} = 0$$

$$\text{Energy:} \quad \rho^0 \frac{De}{Dt} + \frac{\partial}{\partial x}(Pu) = 0$$

$$\text{Equation of State:} \quad P = \mathcal{P}(\varepsilon, \tau)$$

(EOS)

$$\tau \equiv 1/\rho$$

$$\begin{aligned} \rho^0 &= \rho^0(x) \\ &\equiv \rho(x, t=0) \end{aligned}$$

$$e \equiv \varepsilon + (1/2) u^2$$

Specific Internal Energy (SIE)

- With 1-D equations, we can:
 - Test — *rigorously* — fundamental algorithms
 - Quantitatively evaluate algorithm performance





We make some simplifying assumptions.

■ There are two materials.

- Two materials cells (almost) certainly occur during the remap of a multi-material ALE calculation.
- Modeling of two materials requires much more care than one material simulations.
- Modeling of two materials does not imply an unambiguous method for model three (or more) materials.

■ These two materials are described by one velocity.

- This implies — either implicitly or explicitly — that a sub-grid model describes the mixing of the materials within each cell.
- This differs from more sophisticated, multiple velocity-field models that are used, e.g., for two-phase flow.

■ We focus on closure models for pressure equilibration.

- We do not discuss here the important issue of artificial viscosity models for multiple-material cells.



Algorithm I uses the following predictor-corrector approach*.

Predictor

Edge positions: $x_{i+1/2}^{n+1,*} = x_{i+1/2}^n + \Delta t \cdot u_{i+1/2}$

Cell volumes: $V_{i,\text{cell}}^{n+1,*} = x_{i+1/2}^{n+1,*} - x_{i-1/2}^{n+1,*}$

Edge-velocities: $u_{i+1/2}^{n+1,*} = u_{i+1/2}^n - \Delta t (p_{i+1}^n + q_{i+1}^n - p_i^n - q_i^n) / M_{i+1/2,\text{node}}^n$ *Artificial viscosity*

Cell pressure: $p_i^{n+1,*} = p_i^n - \chi \Delta t \rho_i^n (c_{s,i}^{n+1,*})^2 \nabla \cdot u_i^n$ *Adiabatic update*

Corrector

Node mass: $M_{i+1/2,\text{node}} = \frac{1}{2}(M_{i,\text{cell}} + M_{i+1,\text{cell}})$

Edge-velocities: $u_{i+1/2}^{n+1} = u_{i+1/2}^n - \frac{\Delta t}{2} (p_{i+1}^{n+1,*} + q_{i+1}^{n+1,*} - p_i^{n+1,*} - q_i^{n+1,*} + p_{i+1}^n + q_{i+1}^n - p_i^n - q_i^n) / M_{i+1/2,\text{node}}$

Time-center: $u_{i+1/2}^{n+1/2} = \frac{1}{2}(u_{i+1/2}^n + u_{i+1/2}^{n+1})$

Edge positions: $x_{i+1/2}^{n+1} = x_{i+1/2}^n + \Delta t \cdot u_{i+1/2}^{n+1/2}$

Cell volumes: $V_{i,\text{cell}}^{n+1} = x_{i+1/2}^{n+1} - x_{i-1/2}^{n+1}$

Cell density: $\rho_i^{n+1} = M_{i,\text{cell}} / V_{i,\text{cell}}^{n+1} \Rightarrow \tau_i^{n+1} = 1 / \rho_i^{n+1}$

Cell SIE: $\varepsilon_i^{n+1} = \varepsilon_i^n - (\Delta t / \rho_i^n) (p_i^{n+1,*} + q_i^{n+1,*}) ((V_{i+1/2}^{n+1} - V_{i+1/2}^n) / (\Delta t V_{i+1/2}^{n+1}))$

Cell pressure: $p_i^{n+1} = \mathcal{P}(\varepsilon_i^{n+1}, \tau_i^{n+1})$ **Full EOS call**



This algorithm changes for multiple materials.

■ Denote the volume fraction of material α as: $f_\alpha = V_\alpha/V$

■ In the predictor, the change is to the pressure update.

- The pressure of material α at t^n is evaluated: $p_{i,\alpha}^n = \mathcal{P}(\varepsilon_{i,\alpha}^n, \tau_{i,\alpha}^n)$
- Pressure predictor update: $p_{i,\alpha}^{n+1,*} = p_{i,\alpha}^n - \chi \Delta t \rho_{i,\alpha}^n (c_{s,i,\alpha}^n)^2 \nabla \cdot u_i^n$
- With the following relations, Bondarenko & Yanilkin* showed that total energy is conserved in this approach:

$$p_i^{n+1,*} = \sum_{\alpha} \psi_{\alpha} p_{i,\alpha}^{n+1,*} \quad q_i^{n+1,*} = \sum_{\alpha} \psi_{\alpha} q_{i,\alpha}^{n+1,*}$$

where ψ_{α} is determined by the closure model.

■ In the corrector, additional modifications are required.

- The node mass becomes:

$$M_{i+1/2,\text{node}} = \frac{1}{2} \sum_{\alpha} (M_{i,\alpha} + M_{i+1,\alpha}) \quad \text{where} \quad M_{i,\alpha} \equiv f_{i,\alpha} \rho_{i,\alpha} V_i$$



* Bondarenko, Yu.A., Yanilkin, Yu.V., "Computation of thermodynamical parameters of the mixed cells in gas dynamics," VANT (Mathematical Modeling of Physical Processes) 2000;4:12–25 (in Russian).

Additional changes in the corrector are needed.

■ Updated values for material α are as follows:

$$\begin{aligned}
 \text{Volume:} \quad & V_{i,\alpha}^{n+1} = V_{i,\alpha}^n + \Delta t V_{i,\alpha}^{n+1} \nabla \cdot u_{i,\alpha}^{n+1} \\
 \text{Density:} \quad & \rho_{i,\alpha}^{n+1} = M_{i,\text{cell},\alpha} / V_{i,\alpha}^{n+1} \Rightarrow \tau_{i,\alpha}^{n+1} = 1 / \rho_{i,\alpha}^{n+1} \\
 \text{Volume Fraction:} \quad & f_{i,\alpha}^{n+1} = V_{i,\alpha}^{n+1} / V_i^{n+1} \\
 \text{SIE:} \quad & \varepsilon_{i,\alpha}^{n+1} = \varepsilon_{i,\alpha}^n - (\Delta t / \rho_{i,\alpha}^n) (p_{i,\alpha}^{n+1,*} + q_{i,\alpha}^{n+1,*}) \\
 & \quad \times (1/2) (\nabla \cdot u_{i,\alpha}^n + \nabla \cdot u_{i,\alpha}^{n+1,*})
 \end{aligned}$$

- In the above expressions, the following quantities are still undefined:
artificial viscosity $q_{i,\alpha}^n$, velocity divergence $\nabla \cdot u_{i,\alpha}^n$, parameter ψ_α

■ We impose the following constraints:

$$\begin{aligned}
 (1) \text{ Volume:} \quad & V = \sum_{\alpha} V_{\alpha} \Rightarrow \sum_{\alpha} f_{\alpha} = 1 \quad \text{and} \quad \Delta V = \sum_{\alpha} \delta V_{\alpha}, \quad \sum_{\alpha} f_{\alpha} \nabla \cdot u_{\alpha} = \nabla \cdot u \\
 (2) \text{ SIE:} \quad & \varepsilon = \sum_{\alpha} Y_{\alpha} \varepsilon_{\alpha} \quad \text{with} \quad Y_{\alpha} \equiv f_{\alpha} \rho_{\alpha} / \rho, \quad \rho = \sum_{\alpha} f_{\alpha} \rho_{\alpha}
 \end{aligned}$$

■ Assume velocity divergence is modeled as: $\nabla \cdot u_{\alpha} \equiv \lambda_{\alpha} \nabla \cdot u$ such that $\psi_{\alpha} \equiv f_{\alpha} \lambda_{\alpha}$



Algorithm II uses a different approach*.

Node mass: $M_{i+1/2,node} = (1/2)(M_{i,cell} + M_{i+1,cell})$

Time steps: $\Delta t^+ \equiv t^{n+1} - t^n$, $\Delta t^- \equiv t^n - t^{n-1}$

Edge-velocities: $u_{i+1/2}^{n+1/2} = u_{i+1/2}^{n-1/2} - (1/2)(\Delta t^+ + \Delta t^-)(p_{i+1}^n + q_{i+1}^n - p_i^n - q_i^n) / M_{i+1/2,node}$

Edge positions: $x_{i+1/2}^{n+1} = x_{i+1/2}^n + \Delta t^+ \cdot u_{i+1/2}^{n+1/2}$

Cell volumes: $V_{i,cell}^{n+1} = x_{i+1/2}^{n+1} - x_{i-1/2}^{n+1}$

Cell density.: $\rho_i^{n+1} = M_{i,cell} / V_{i,cell}^{n+1} \Rightarrow \tau_i^{n+1} = 1 / \rho_i^{n+1}$

Cell SIE: $\varepsilon_i^{n+1} = \varepsilon_i^n - (1/2)(p_i^{n+1} + q_i^{n+1} - p_i^n - q_i^n)(\tau_i^{n+1} - \tau_i^n)$

Cell pressure: $p_i^{n+1} = \mathcal{P}(\varepsilon_i^{n+1}, \tau_i^{n+1})$ **Full EOS call**

These are implicit, nonlinear equations in ε_i^{n+1} and p_i^{n+1} that are solved with an iterative solution procedure.

■ For multiple materials, Alg. II changes similarly to Alg. I



Algorithm III is similar to the first algorithm*.

Predictor

Edge positions: $x_{i+1/2}^{n+1/2} = x_{i+1/2}^n + (\Delta t/2) u_{i+1/2}^n$

Cell volumes: $V_{i,\text{cell}}^{n+1/2} = x_{i+1/2}^{n+1/2} - x_{i-1/2}^{n+1/2}$

Cell specific vol.: $\tau_i^{n+1/2} = V_{i,\text{cell}}^{n+1/2} / M_{i,\text{cell}}$

Cell pressure: $p_i^{n+1/2} = p_i^n - \left((c_{s,i}^n)^2 / \tau_i^n \right) \left(\delta V_i^{n+1/2} / V_i^n \right)$

Adiabatic update

Corrector

Edge-velocities: $u_{i+1/2}^{n+1} = u_{i+1/2}^n - \frac{\Delta t}{M_{i+1/2,\text{node}}} (p_i^{n+1/2} + q_i^{n+1/2} - p_i^{n+1/2} - q_i^{n+1/2})$

Edge positions: $x_{i+1/2}^{n+1} = x_{i+1/2}^n + \Delta t (u_{i+1/2}^n + u_{i+1/2}^{n+1}) / 2$

Cell volumes: $V_{i,\text{cell}}^{n+1} = x_{i+1/2}^{n+1} - x_{i-1/2}^{n+1}$

Cell specific vol.: $\tau_i^{n+1} = V_{i,\text{cell}}^{n+1} / M_{i,\text{cell}}$

Cell SIE: $\varepsilon_i^{n+1} = \varepsilon_i^n - \left((p_i^{n+1} + q_i^{n+1}) \delta V_i^{n+1} / M_{i,\text{cell}} \right)$

Cell pressure: $p_i^{n+1} = \mathcal{P}(\varepsilon_i^{n+1}, \tau_i^{n+1})$

Artificial viscosity



* Kamm J.R., Shashkov M.J., Rider, W.J., "A new pressure relaxation closure model for one-dimensional two-material Lagrangian hydrodynamics, *Eur. Phys. J. Web Conf.* 2011, doi:10.1051/epjconf/201010000038.

With Alg. I, several closure models for pressure equilibration can be examined.

① **Equal compressibility***: $\nabla \cdot u_\alpha = \nabla \cdot u$ so $\lambda_\alpha = 1$, $\psi_\alpha = f_\alpha$

- Assume this is valid at the predictor step: $\nabla \cdot u_\alpha^{n+1/2} = \nabla \cdot u^{n+1/2}$
- Easy to implement; computationally efficient: $p = \sum f_\alpha p_\alpha$
- Physically incorrect—with questionable results—in many situations.
 - E.g., cell with gas (highly compressible) and metal (low compressibility).

② **Equal pressure†**: $p_1 = p_2$ and $q_1 = q_2$

- This is the result of instantaneous (i.e., over Δt) pressure equilibration.

- Leads to coupled equations: one must solve for ΔE_α , ΔV , $p^{n+1/2}$ in:

$$\Delta E_\alpha = (p^{n+1/2} + q^n) \mu \Delta V_\alpha, \quad \Delta V = \sum \Delta V_\alpha, \quad p^{n+1/2} = \mathcal{P}\left(\frac{M_\alpha}{V_\alpha^n + \Delta V_\alpha}, \frac{E_\alpha + \Delta E_\alpha}{M_\alpha}\right)$$

where $\mu \equiv (\nabla \cdot u^n + \nabla \cdot u^{n+1}) V^n \Delta t / (2 \Delta V)$

- These imply expressions for updated SIE and volume fraction:

$$\varepsilon_\alpha^{n+1/2} = \varepsilon_\alpha + (\Delta E_\alpha / M_\alpha), \quad f_\alpha^{n+1/2} = (V_\alpha + \Delta V_\alpha) / (V + \Delta V)$$

- Bakhrah, S., Spiridonov, V., Shanin, A., "A method for computing gas-dynamic flows of inhomogeneous medium in Lagrangian-Eulerian coordinates," *DAN SSR* 1984;276:829–833 (in Russian; translated in *Sov. Phys. Doklady* 1984;29:443–445).

- † Harlow, F., "The particle-in-cell computing method for fluid dynamics," in Alder, B., Fernbach, S., Rotenberg, M., eds., *Methods in Computational Physics*, Vol. 3; New York: Academic Press; 1964, 319–343; Zharova, G.V., Yanilkin, Yu.V. "The EGAK code mixed cell pressure equilibration algorithm," *VANT (Mathematical Modeling of Physical Processes)* 1993;3:77–81 (in Russian).



Equal-increment models can also be formulated.

③ Equal pressure increments* (ΔP):

- Assume that the general acoustic approximation is valid:

$$\partial P / \partial t = (\partial P / \partial \rho)(\partial \rho / \partial t) = \rho c^2 \nabla \cdot u$$

- Assume that this quantity has the same value for all materials:

$$\rho_1 c_1^2 \nabla \cdot u_1 = \rho_2 c_2^2 \nabla \cdot u_2$$

- This leads to the following closed-form expressions:

$$\nabla \cdot u_{\alpha}^n = \lambda_{\alpha} \nabla \cdot u^n \quad \text{where} \quad \lambda_{\alpha} \equiv \frac{1}{\rho_{\alpha}^n (c_{\alpha}^n)^2} \left(\sum \frac{f_{\beta}^n}{\rho_{\beta}^n (c_{\beta}^n)^2} \right)^{-1}$$

④ Equal velocity increments[†] (Δv):

- One velocity per cell, so equal velocity *increments* is plausible.
- Acoustic approximation implies: $\nabla \cdot u_{\alpha} \approx -(\delta \rho_{\alpha}) / (\rho_{\alpha} \Delta t) \approx -(\delta u_{\alpha}) / (c_{\alpha} \Delta t)$
- This leads to the following closed-form expressions:

$$\nabla \cdot u_{\alpha}^n = \lambda_{\alpha} \nabla \cdot u^n \quad \text{where} \quad \lambda_{\alpha} \equiv \frac{1}{c_{\alpha}^n} \left(\sum (f_{\beta}^n / c_{\beta}^n) \right)^{-1}$$

* Bondarenko, Yu.A., Yanilkin, Yu.V., "Computation of thermodynamical parameters of the mixed cells in gas dynamics," VANT (Mathematical Modeling of Physical Processes) 2000;4:12–25 (in Russian).

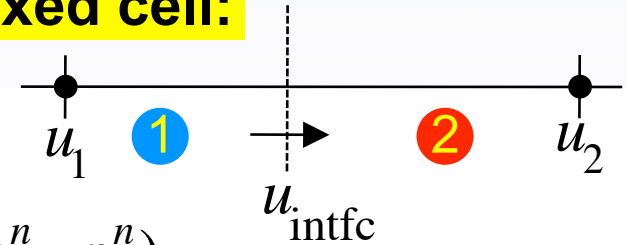
† Goncharov, E.A., Yanilkin, Yu.V., "New method for computations of thermodynamical states of the materials in mixed cells," VANT (Mathematical Modeling of Physical Processes) 2004;3:16–30 (in Russian).



With Alg. II, a linearized Riemann problem* (LRP) used.

⑤ Consider a Riemann problem in the mixed cell:

- Riemann invariants imply the well-known **linearized** contact velocity expression:



$$u_{\text{intfc}}^{n+1/2} = \frac{(\rho c_s)_1^n u_1^{n+1/2} + (\rho c_s)_2^n u_2^{n+1/2} + (p_1^n - p_2^n)}{(\rho c_s)_1^n + (\rho c_s)_2^n}$$

- From Algorithm II, the following update for the density follows:

$$\frac{1}{\rho^{n+1}} - \frac{1}{\rho^n} = \Delta t^+ \frac{u_i^{n+1/2} - u_{i-1}^{n+1/2}}{M}$$

- Combining these equations gives updates for each material implies:

$$\frac{1}{\rho_1^{n+1}} - \frac{1}{\rho_1^n} = \frac{\Delta t}{M_1} \left[\frac{(\rho c_s)_2^n}{(\rho c_s)_1^n + (\rho c_s)_2^n} (u_i^{n+1/2} - u_{i-1}^{n+1/2}) + \frac{p_1^n - p_2^n}{(\rho c_s)_1^n + (\rho c_s)_2^n} \right]$$

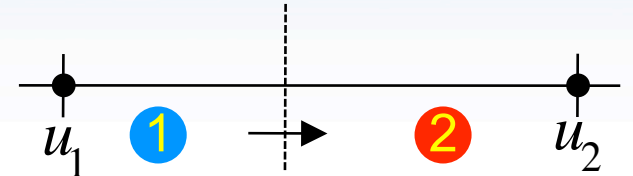
$$\frac{1}{\rho_2^{n+1}} - \frac{1}{\rho_2^n} = \frac{\Delta t}{M_2} \left[\frac{(\rho c_s)_1^n}{(\rho c_s)_1^n + (\rho c_s)_2^n} (u_i^{n+1/2} - u_{i-1}^{n+1/2}) - \frac{p_1^n - p_2^n}{(\rho c_s)_1^n + (\rho c_s)_2^n} \right]$$

- Delov, V., Sadchikov, V.V., "Comparison of several models for computation of thermodynamical parameters for heterogeneous Lagrangian cells," VANT (Mathematical Modeling of Physical Processes) 2005;1:57–70 (in Russian).¹²



The LRP* method also involves additional equations.

- From $\nabla \cdot u \approx \Delta V / (V \Delta t)$, the individual velocity divergences are obtained:



$$\nabla \cdot u_{\alpha}^n = (\lambda_{\alpha} / f_{\alpha}^n) \nabla \cdot u^n + \omega^n [(p_{\alpha}^n - p_{\Sigma}^n) / (f_{\alpha}^n h^n)] \cdot [(\rho c)_{\Sigma}^n]^{-1}$$

where

$$p_{\Sigma}^n \equiv \frac{1}{2}(p_1^n + p_2^n), \quad (\rho c)_{\Sigma}^n \equiv \frac{1}{2}[(\rho c)_1^n + (\rho c)_2^n], \quad \lambda_{\alpha} \equiv 1 - \left[\frac{1}{2}(\rho c)_1^n / (\rho c)_{\Sigma}^n \right],$$

with h^n a characteristic mesh size and ω^n improves stability:

$$\omega^n \equiv \left\{ \frac{1}{2}[(\rho c)_1^n + (\rho c)_2^n] \right\}^2 \left\{ \rho^n [(\rho c^2)_1^n + (\rho c^2)_2^n] \right\}^{-1} \min \{ f_1^n, f_2^n \}$$

- From the velocity divergence equation, the volume change is:

$$V_{\alpha}^{n+1} - V_{\alpha}^n = \lambda_{\alpha} (V^{n+1} - V^n) + (\omega \Delta t V^n / h) (p_{\alpha}^n - p_{\Sigma}^n) [(\rho c)_{\Sigma}^n]^{-1}$$

- After some algebra, this implies that the energy update for material α is modified by an additional term:

$$\Delta \varepsilon_{\alpha}^{n+1} = [(\omega^n \tau) / (\rho^n h^n)] f_{\alpha} [p_1^n (p_1^n - p_{\Sigma}^n) + p_2^n (p_2^n - p_{\Sigma}^n)] [(\rho c)_{\Sigma}^n]^{-1}$$



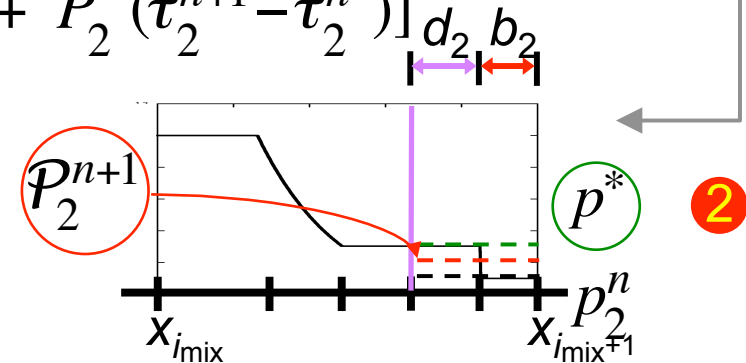
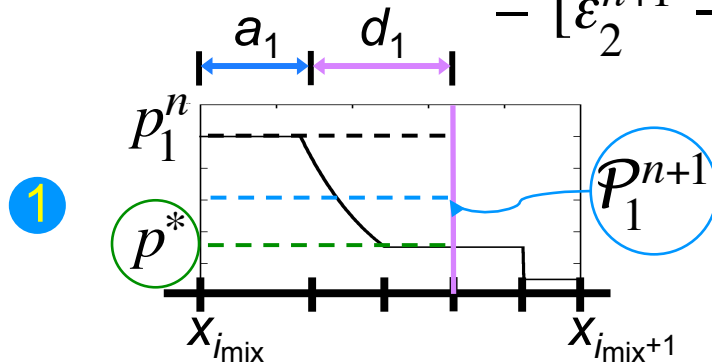
- Delov, V., Sadchikov, V.V., "Comparison of several models for computation of thermodynamical parameters for heterogeneous Lagrangian cells," *VANT (Mathematical Modeling of Physical Processes)* 2005;1:57–70 (in Russian).¹³

Kamm & Shashkov* (KS) break the pressure equilibration assumption of Després† using local Riemann problem solutions.

- Pressure relaxation in the mixed cell reduces to the solution of a minimization problem in $\tau_1^{n+1}, \varepsilon_1^{n+1}, \tau_2^{n+1}, \varepsilon_2^{n+1}$

$$\min_{\{\tau_1^{n+1}, \varepsilon_1^{n+1}, \tau_2^{n+1}, \varepsilon_2^{n+1}\}} f_0 \equiv \|\mathcal{P}_1^{n+1} - p_1^{RP}\| + \|\mathcal{P}_2^{n+1} - p_2^{RP}\|$$

$$\text{subject to: } \begin{cases} 0 = f_1 \equiv c_1 \tau_1^{n+1} + c_2 \tau_2^{n+1} - \tau^{n+1} \\ 0 = f_2 \equiv c_1 \varepsilon_1^{n+1} + c_2 \varepsilon_2^{n+1} - \varepsilon^{n+1} \\ 0 = f_3 \equiv \varepsilon_1^{n+1} - \varepsilon_1^n + P_1 (\tau_1^{n+1} - \tau_1^n) \\ \quad - [\varepsilon_2^{n+1} - \varepsilon_2^n + P_2 (\tau_2^{n+1} - \tau_2^n)] \end{cases}$$



Mixed-cell Riemann Problem

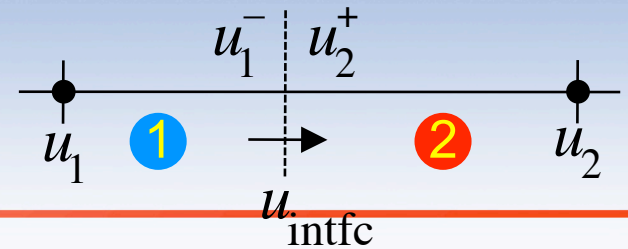
- Complicated — and untested for realistic problems in multi-D.

• Kamm J.R., Shashkov M.J., *Comm. Comput. Phys.*, 2010; 7:927–976.

† Després, B., Lagoutière, F., *Prog. Comput. Fluid Dyn.* 2007; 7:295–310.



Kamm, Shashkov & Rider* (KSR) also propose a linearized Riemann model.



- Inspired by VNIIEF work, KSR used the linearized Riemann problem to update the materials' volumes, volume fractions, and SIEs.

- There is a problem: this SIE update is *not consistent* with the total work done on the mixed cell, i.e., $\sum_k M_k d\varepsilon_k^{n+1,*} \neq -p_{i_{\text{mix}}+1/2}^{n+1/2} dV_{i_{\text{mix}}+1/2}^{n+1}$
- Let $d\tilde{\varepsilon}_k$ be the change in SIE that guarantees consistency:

$$\text{Consistent} \quad \boxed{\varepsilon_k^{n+1}} = \boxed{\varepsilon_k^{n+1,*}} + \boxed{d\tilde{\varepsilon}_k} \quad \text{Known} + \text{Unknown}$$

- Assume that the pressure change due to $d\tilde{\varepsilon}_k$: (1) is the same for both materials, and (2) depends *only* on the energy (*not* on the density).
- Using the expression for the total SIE discrepancy and the thermodynamic derivatives $(\partial p_k / \partial \varepsilon_k)_{\rho_k}$, one can solve for the corrections to the SIEs and then update the pressures:

$$\varepsilon_k^{n+1} = \varepsilon_k^{n+1,*} + d\tilde{\varepsilon}_k \quad \text{and} \quad p_k^{n+1} = \mathcal{P}_k(\varepsilon_k^{n+1}, \tau_k^{n+1})$$



• Kamm J.R., Shashkov M.J., Rider, W.J., "A new pressure relaxation closure model for one-dimensional two-material Lagrangian hydrodynamics, *Eur. Phys. J. Web Conf.* 2011, doi:10.1051/epjconf/201010000038.

Tipton's method is a widely used, robust multi-material, pressure relaxation for multi-D.

- **Assumption #1:** Predictor pressure based on adiabatic update:

$$p_k^{n+1/2} = p_k^n - \left[(cs_k^n)^2 / \tau_k^n \right] \boxed{\delta V_k^{n+1/2} / V_k^n}$$

Unknown

- **Assumption #2:** There is a relaxation term added to each material's pressure, so that these sums are all equal:

Predictor pressure of k-th material $p_k^{n+1/2} + \boxed{R_k}$ $=$ $\boxed{\hat{p}^{n+1/2}}$ *Overall predictor pressure*

where $\boxed{R_k} = - \left(cs_k^n / \tau_k^n \right) \left(L^n / \delta t \right) \boxed{\delta V_k^{n+1/2} / V_k^n}$ *Relaxation term for k-th material*

Unknown

- **Assumption #3:** Volume changes add up correctly:

$$\sum_k \boxed{\delta V_k^{n+1/2}} = V^{n+1/2}$$

Total predictor volume change is known from standard algorithm

- One can solve for $\boxed{\hat{p}^{n+1/2}}$ and $\boxed{\delta V_k^{n+1/2}}$ in closed form.

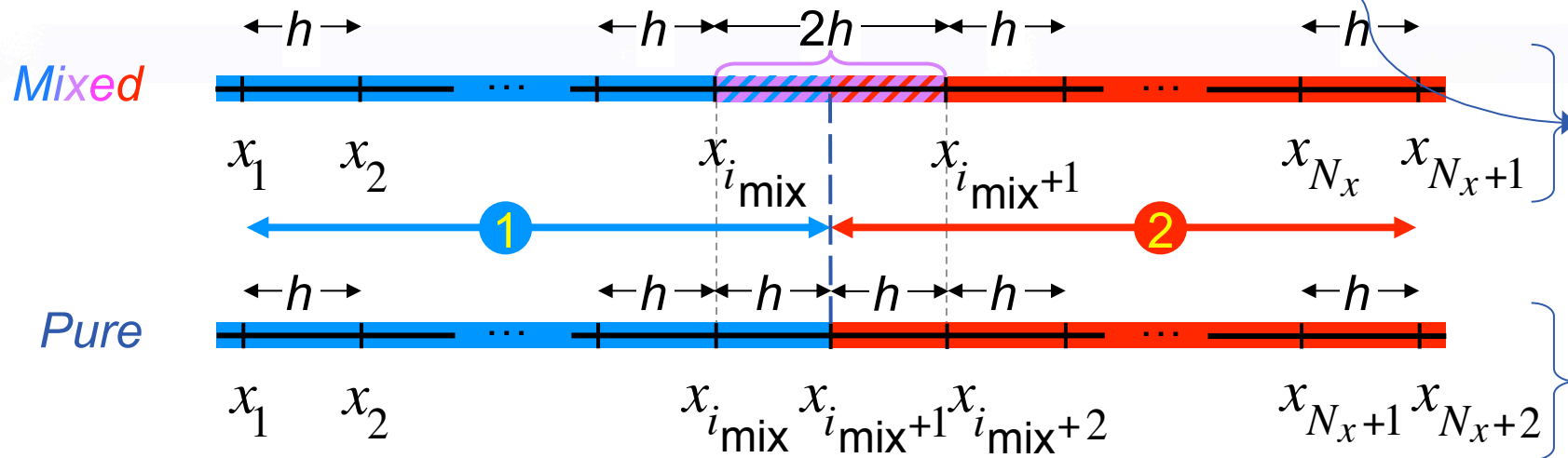
- The second step of a two-step time-integrator uses this information to obtain the final updated values.



The initializations of the pure-material and mixed-cell test problems are as follows.

■ The test problems were run similarly:

- N_x zones on $x_{\min} \leq x < x_{\max}$ with $\Delta x_i = h$, $i \neq i_{\text{mix}}$
- One mixed cell for $i = i_{\text{mix}}$ with $\Delta x_{i_{\text{mix}}} = 2h$



- The fictitious **mixed**-cell interface is at the center of mixed cell of width $2h$, with no explicit mass-matching.

- We compare these results with **pure**-material calculations that have the actual interface.

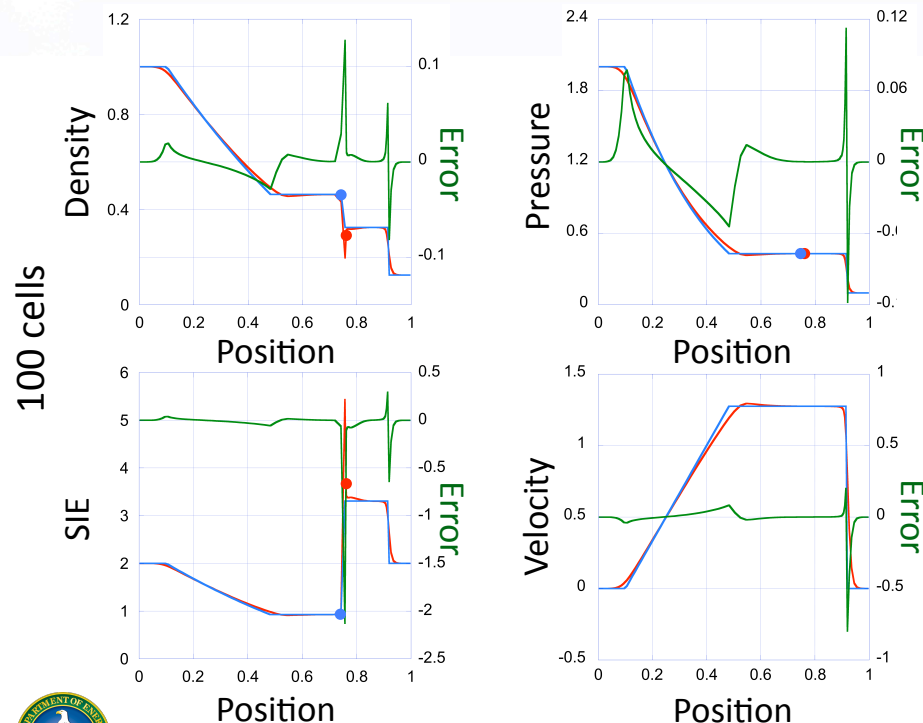


Test Problem #1: Modified Sod Shock Tube

- Two-gas, low Mach number shock tube initial conditions:

$$(\rho, p, u, \gamma) = \begin{cases} (1.0, 2.0, 0.0, 2.0), & 0 \leq x < 0.5, \text{ Material 1} \\ (0.125, 0.1, 0.0, 1.4), & 0.5 < x \leq 1.0, \text{ Material 2} \end{cases} \quad t_{\text{final}} = 0.2$$

- Final-time snapshots show the standard shock-tube evolution.



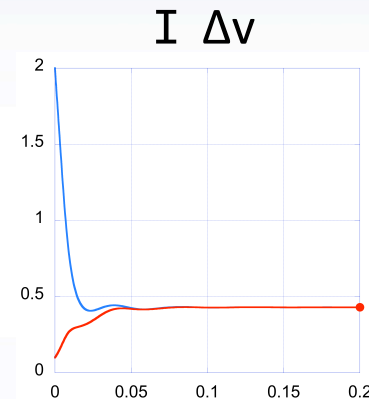
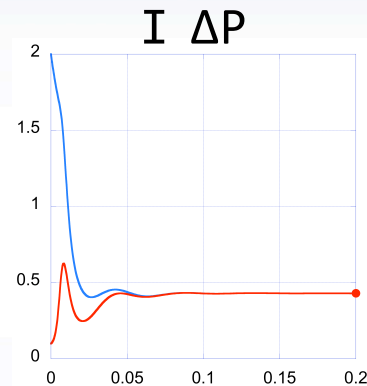
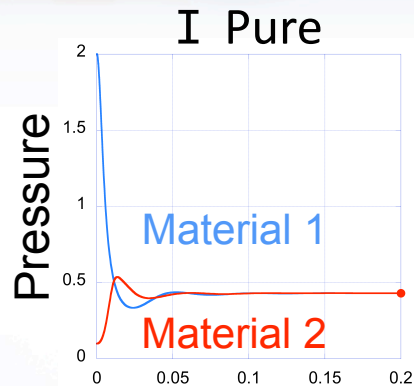
- In the following slides, we present time-histories in the single **mixed** cell.
- Results for all of the methods mentioned are presented.

- All methods have been demonstrated to be about first-order accurate on this problem.

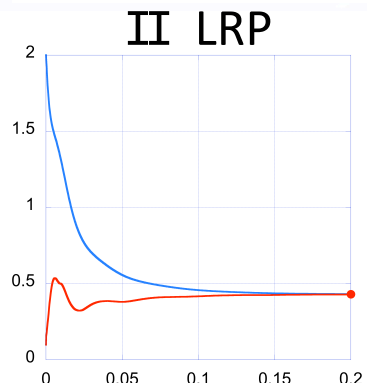
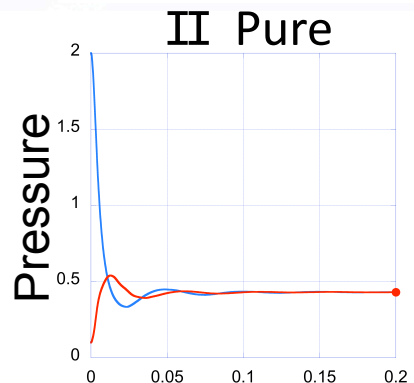


"Closed-form" – Computed = Error

Modified Sod Pressure History

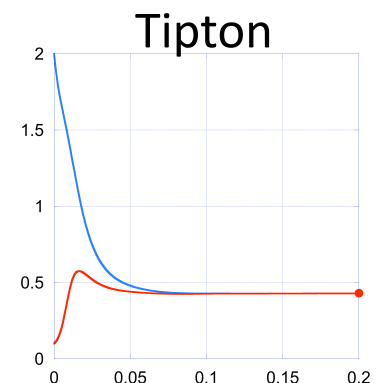
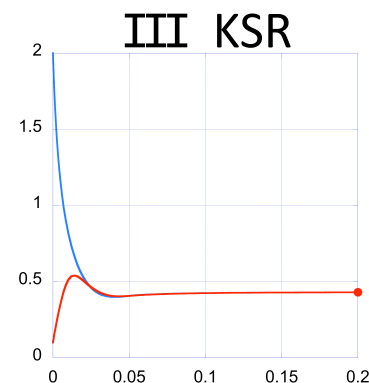
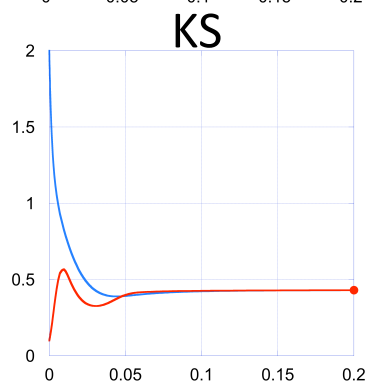
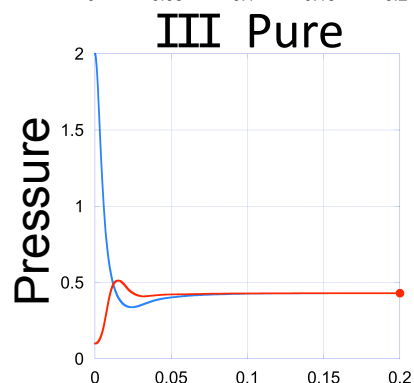


- All methods:
 - Equilibrate
 - Obtain the correct final pressure

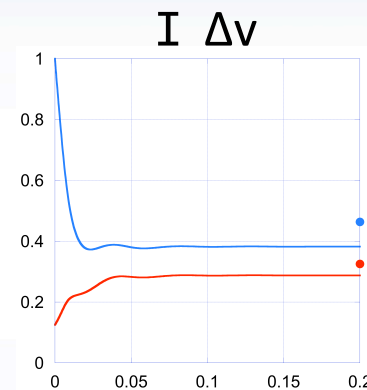
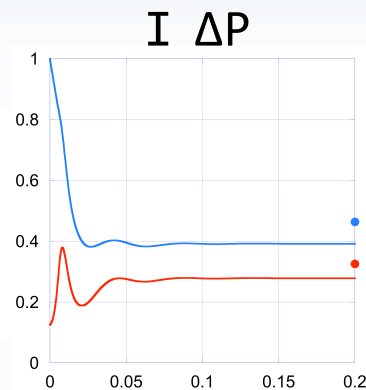
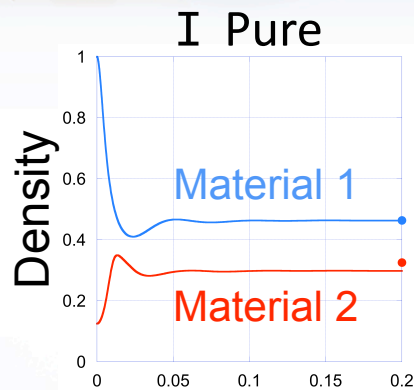


- All methods exhibit pressure oscillations, also.

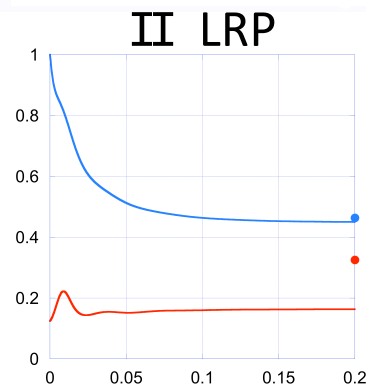
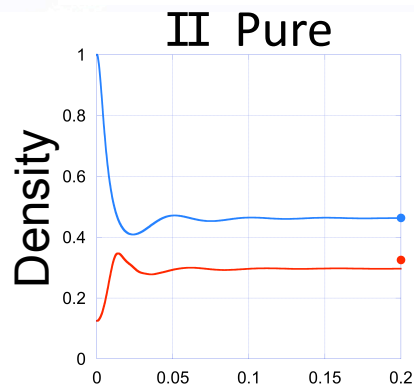
- Among mixed cell methods, KSR and Tipton look heuristically the “nicest.”



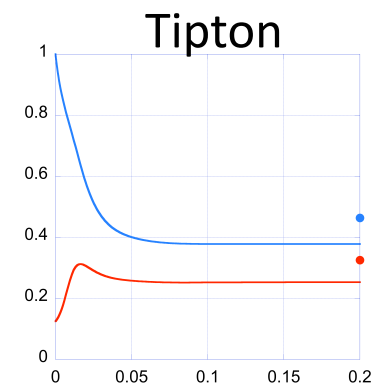
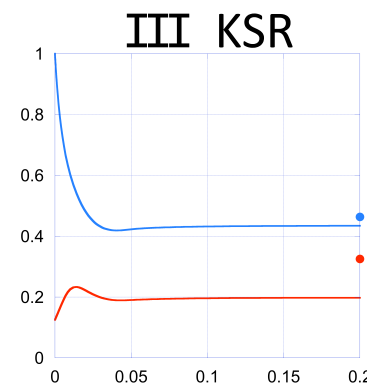
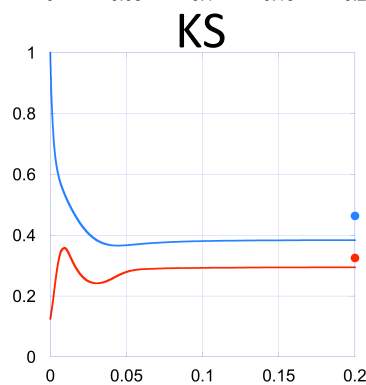
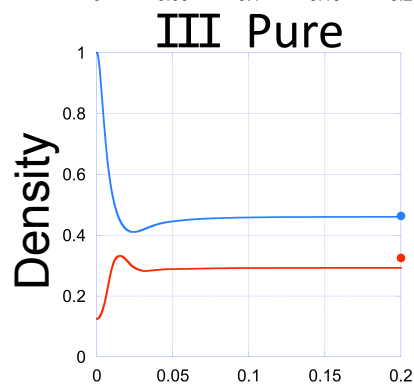
Modified Sod Density History



- The “**pure**” methods come closest to the correct values at the final time.

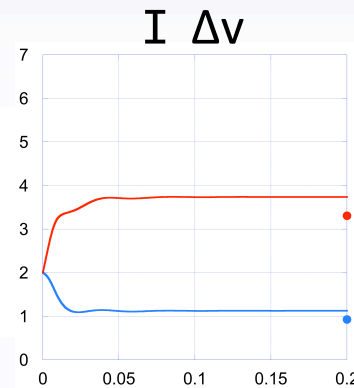
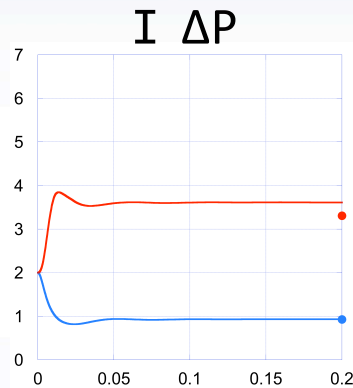
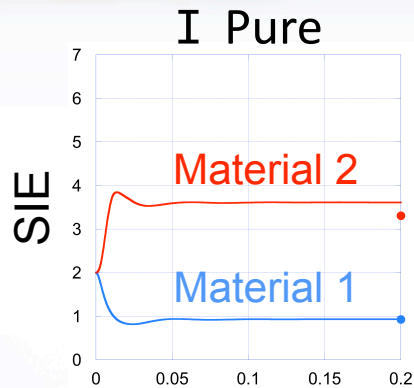


- All **mixed** cell methods undershoot the final values.
- Which method looks heuristically the “best”?

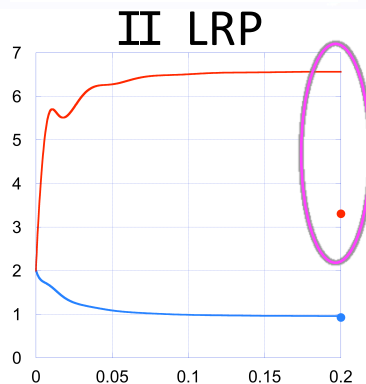
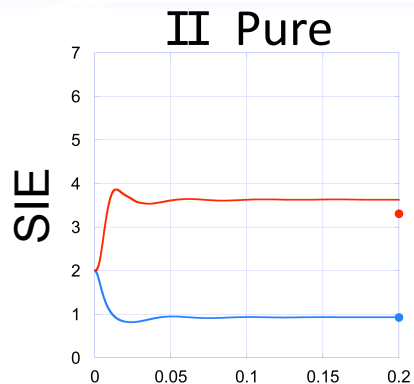


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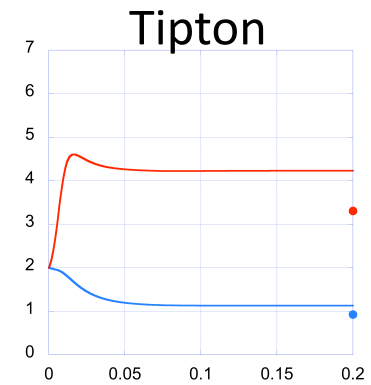
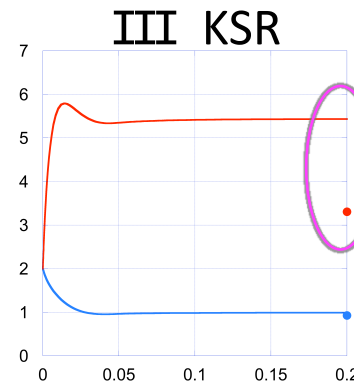
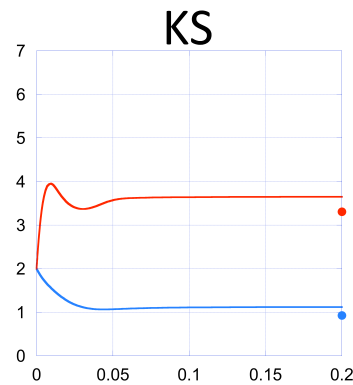
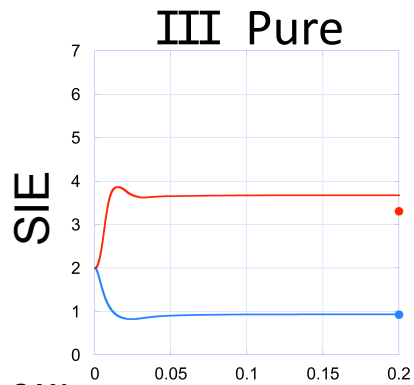
Modified Sod Specific Internal Energy History



- For **material 1**, all methods perform about equally well, and get the correct result.



- For **material 2**, both linearized Riemann problem methods overshoot significantly.
- Tipton overshoots a little, too.
- KS heuristically the “best”?

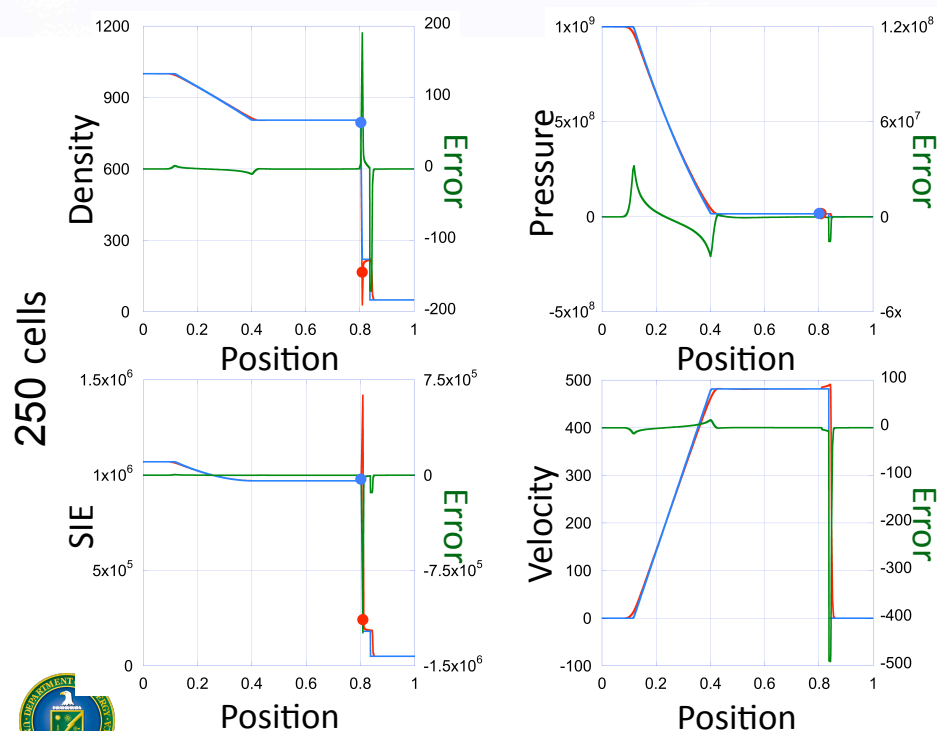


Test Problem #2: the Water-Air Shock Tube

Water-air shock tube* initial conditions:

$$(\rho, p, u, \gamma, p_\infty) = \left\{ \begin{array}{ll} (1.e+3, 1.e+9, 0.0, 4.4, 6.e+8), & 0 \leq x < 0.7, \text{ Material 1} \\ (5.e+1, 1.e+6, 0.0, 1.4, 0.0), & 0.7 < x \leq 1.0, \text{ Material 2} \end{array} \right\} \quad \begin{array}{l} p = (\gamma - 1)\rho\varepsilon - \gamma p_\infty \\ t_{\text{final}} = 2.2e-4 \end{array}$$

Final-time snapshots show the stronger shock-tube evolution.



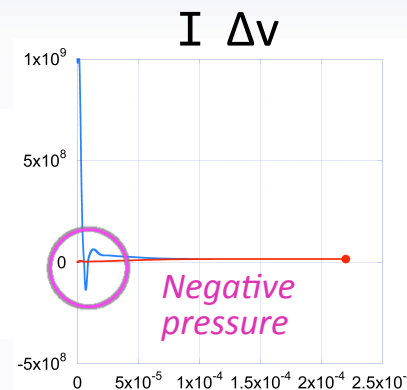
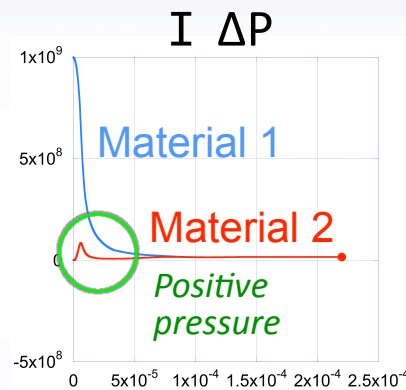
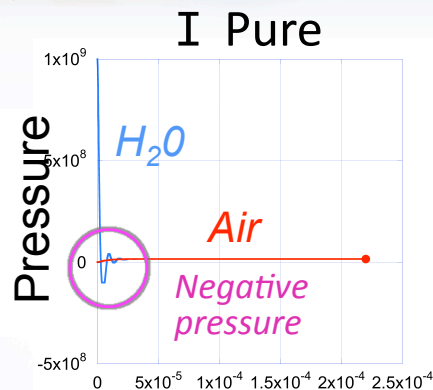
- In the following slides, we present time-histories in the single **mixed** cell.
- Results for all of the methods mentioned are presented.

All methods have been demonstrated to be about first-order accurate on this problem.

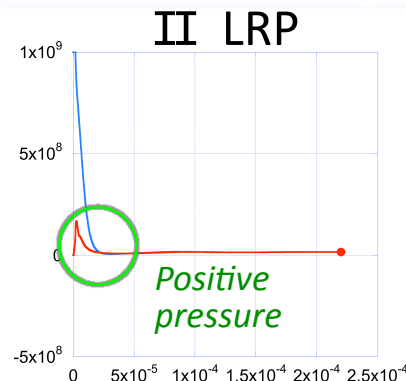
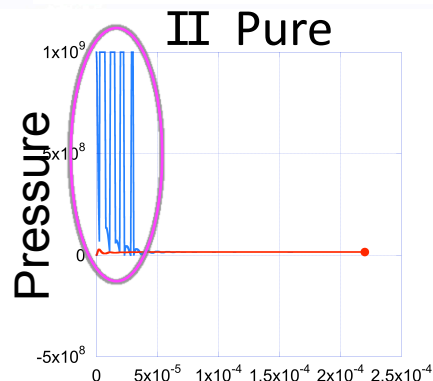
* R. Saurel & R. Abgrall, "A Multiphase Godunov Method for Compressible Multifluid and Multiphase Flows," *J. Comput. Phys.* 1999; **150**:425–467.



Water-Air Pressure History

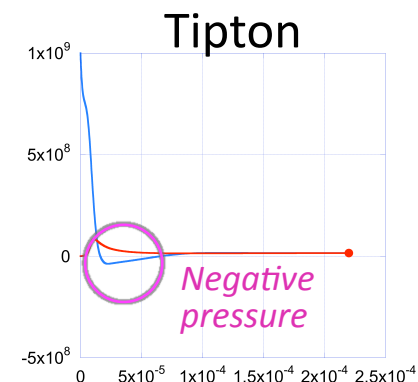
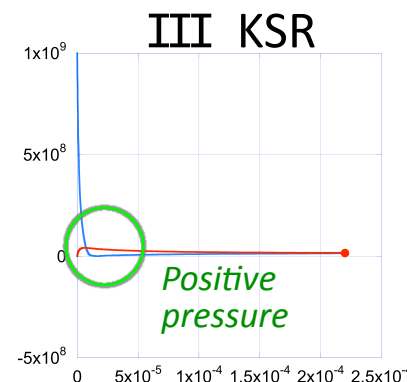
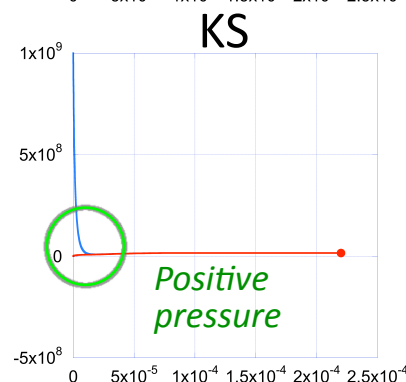
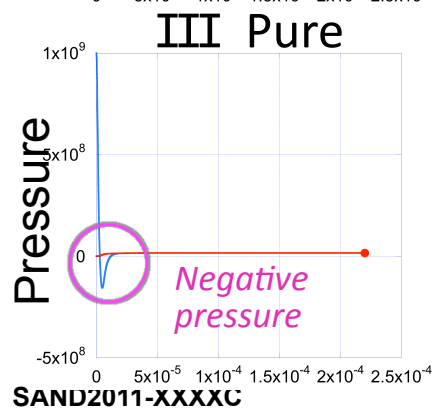


- All methods:
 - Equilibrate
 - Obtain the correct final pressure



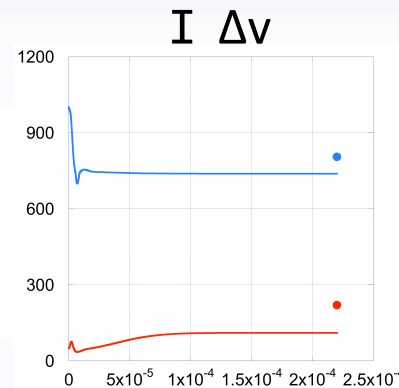
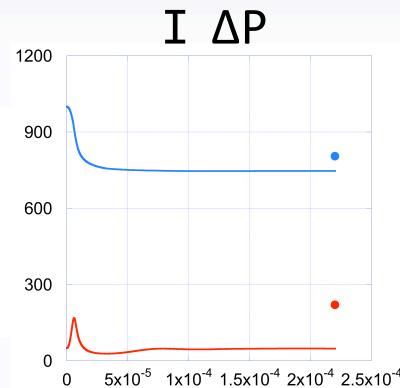
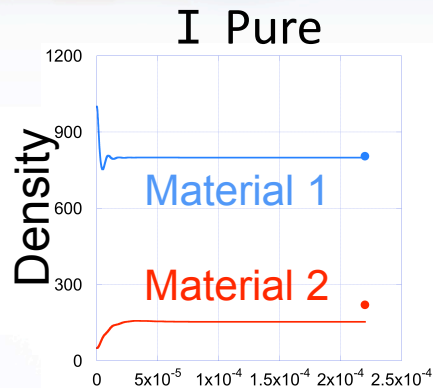
- Some pure and mixed cell methods have negative pressure.

- The mixed cell methods based on Riemann problems have no negative pressure.

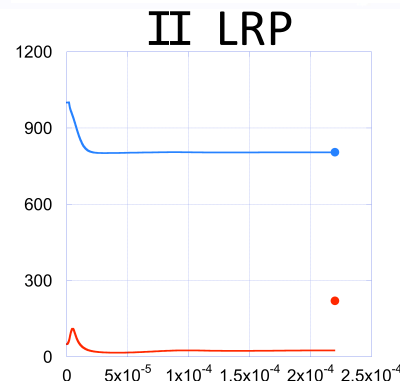
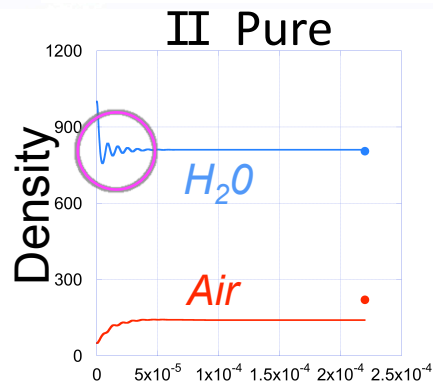


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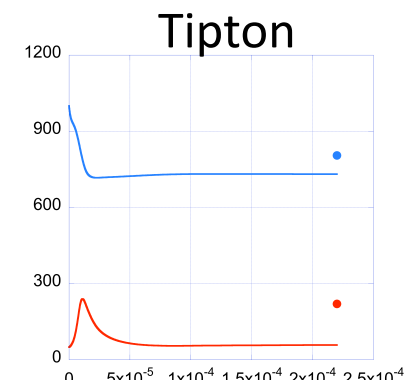
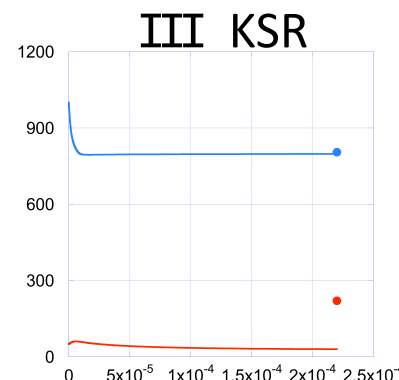
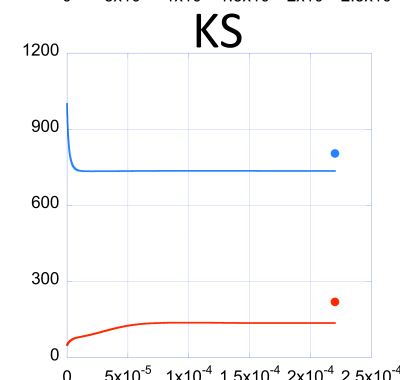
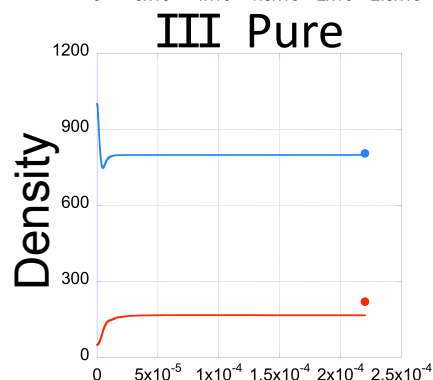
Water-Air Density History



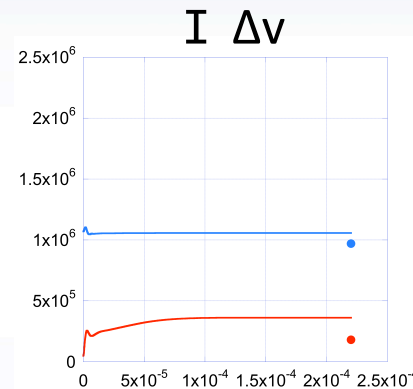
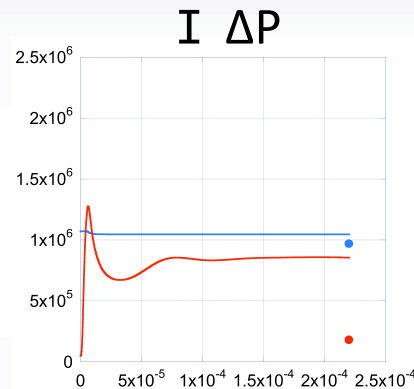
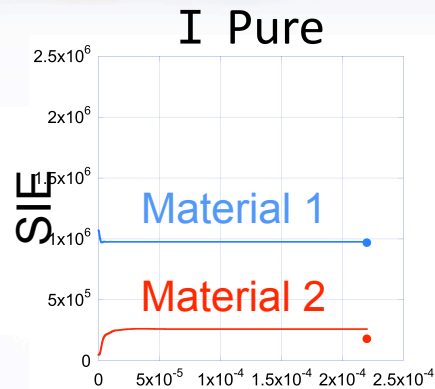
- The “**pure**” methods come closest to the correct values at the final time.



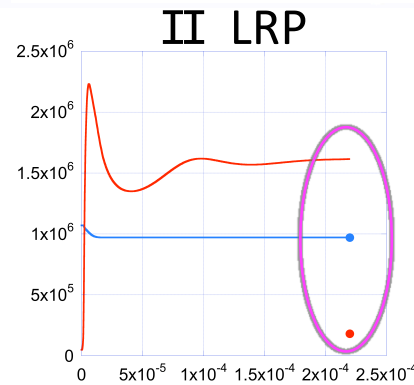
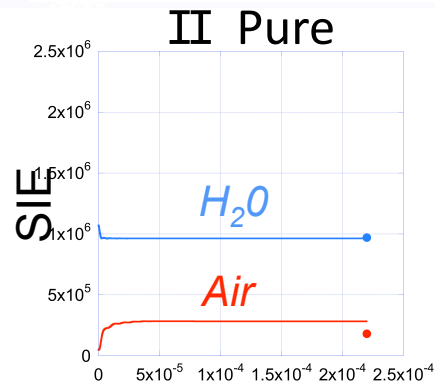
- For **material 2**, **mixed** cell methods consistently undershoot final values more than **pure** methods.
- Which method looks heuristically the “best”?



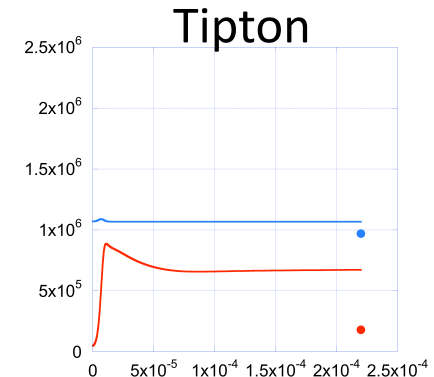
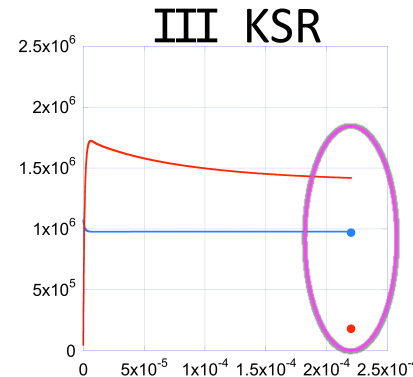
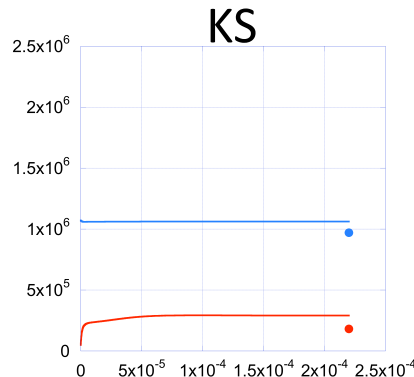
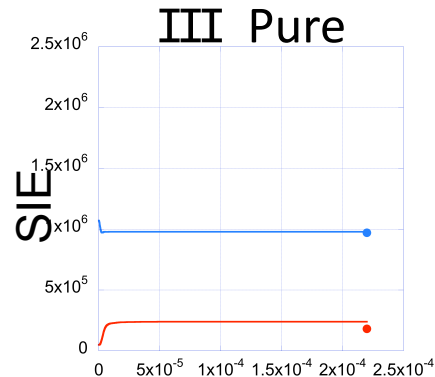
Water-Air Specific Internal Energy History



- For **material 1**, all methods are about the same, close to the exact final value.



- For **material 2**, both linearized Riemann problem methods overshoot seriously.
 - Tipton, ΔP overshoot **material 2**.
 - KSR has volume fraction “flip.”





Summary of these results

■ Pure Material:

- Basic algorithm with no mixed cell; straightforward for ideal problems.

⊕ No mixed cell assumptions.

⊖ No mixed cell assumptions.

■ Equal ΔP :

- Acoustic approximation, assumed to be equal for all materials.

⊕ Closed-form expressions, 2-D.

⊖ Sometimes oscillatory, less accurate SIE.

■ Equal Δv :

- Single velocity → equal velocity increments is a plausible assumption.

⊕ Closed-form expressions, 2-D.

⊖ Sometimes oscillatory, negative pressure.

■ Linearized Riemann Problem (LRP):

- Linearized Riemann problem in mixed cell is used as conservative closure.

⊕ “Physics-based”, 2-D.

⊖ Questionable SIE, volume fractions.

■ Kamm & Shashkov (KS):

- Full Riemann problem in mixed cell → “optimal” pressure of each material.

⊕ Physics-based.

⊖ Complicated. 2-D? Strength?

■ Kamm, Shashkov & Rider (KSR):

- Linearized Riemann problem in mixed cell is used as conservative closure.

⊕ “Physics-based”, 2-D.

⊖ Questionable SIE, volume fractions.

■ Tipton:

- Relaxation term → equal pressures: solve *exactly* for this term.

⊕ Robust, fast, 2-D & strength.

⊖ Rough & ready assumptions, good results.



- There is no clear “fixation” answer to the methods





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