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A New Pressure Relaxation Closure Model for Two-Material Lagrangian Hydrodynamics

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Outline of this talk

- 1-D, two-material Lagrangian hydrodynamics
- The closure problem and pressure relaxation
- Interpretation of the approach of Delov & Sadchikov and Goncharov & Yanilkin
- Test problem results
- Summary, conclusions, and future work

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

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

Momentum: $$\rho \frac{du}{dt} + \frac{dP}{dx} = 0 \qquad \tau \equiv 1/\rho \ , \ P = \mathcal{P}(\varepsilon,\tau)$$

Specific Internal Energy (SIE)

Energy: $$\rho_k \frac{d\varepsilon_k}{dt} + P_k \frac{du_k}{dx} = 0 \Leftrightarrow M_k \, d\varepsilon_k + P_k \, dV_k = 0$$

  - Mass of each fluid parcel is conserved
  - Cell edges evolve with the trajectory equation: $dx_i/dt = u_i$

- With the 1-D equations, we can:
  - Test fundamental algorithms
  - Rigorously evaluate algorithm performance quantitatively

- Extensibility to <u>2-D</u> and <u>material</u> <u>strength</u> are important.

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We consider a basic Lagrangian predictor-corrector method for pure cells.

Predictor

Edge positions: $x_i^{n+1/2} = x_i^n + (\delta t/2)\ u_i^n$

Cell volumes: $V_i^{n+1/2} = x_{i+1}^{n+1/2} - x_i^{n+1/2}$

Cell specific vol.: $\tau_{i+1/2}^{n+1/2} = V_{i+1/2}^{n+1/2} \big/ M_{i+1/2}$

Cell pressure: $p_{i+1/2}^{n+1/2} = p_{i+1/2}^n - \left((c_{s,i+1/2}^n)^2 \big/ \tau_{i+1/2}^n \right) \left(\delta V_{i+1/2}^{n+1/2} \big/ V_{i+1/2}^n \right)$

Adiabatic update

Corrector

Edge-velocities: $u_i^{n+1} = u_i^n - \frac{\delta t}{m_i} (p_{i+1/2}^{n+1/2} - p_{i-1/2}^{n+1/2})$

Edge positions: $x_i^{n+1} = x_i^n + \delta t\ (u_i^n + u_i^{n+1}) \big/ 2$

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

Cell specific vol.: $\tau_{i+1/2}^{n+1} = V_{i+1/2}^{n+1} \big/ M_{i+1/2}$

Cell SIE: $\varepsilon_{i+1/2}^{n+1} = \varepsilon_{i+1/2}^n - \left(p_{i+1/2}^{n+1}\ \delta V_{i+1/2}^{n+1} \big/ M_{i+1/2} \right)$

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

Full EOS call

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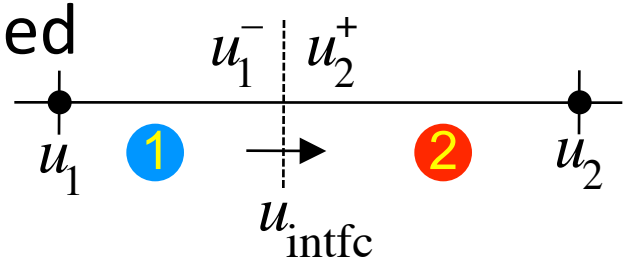
Sub-scale model, motivated by Delov & Sadchikov* and Goncharov & Yanilkin§…



- *Assumption #1*: Interface velocity is from the linearized Riemann solver

$$u_{\text{intfc}} = \frac{\rho_1\, c_{s,1}\, u_1^- + \rho_2\, c_{s,2}\, u_2^+ + (p_1 - p_2)}{\rho_1\, c_{s,1} + \rho_2\, c_{s,2}}$$

- *Assumption #2*: Sub-cell velocity is linear in x

$$u_1^- = u_2^+ = f_2\, u_1 + f_1\, u_2$$

Volume fraction

- #1 + #2 $\Rightarrow$

$$u_{\text{intfc}} = f_2\, u_1 + f_1\, u_2 + \frac{\Delta p_{1,2}}{\kappa_1 + \kappa_2}$$

- Materials' volume changes are related to velocities:

$$\delta V_1 = (u_{\text{intfc}} - u_1)\,\delta t \;,\quad \delta V_2 = (u_2 - u_{\text{intfc}})\,\delta t$$

- Together, these imply:

$$\begin{cases} \delta V_1 = f_1\, \delta V + \frac{1}{2}(\Delta p_{1,2} / \bar{\kappa})\,\delta t \\ \delta V_2 = f_2\, \delta V - \frac{1}{2}(\Delta p_{1,2} / \bar{\kappa})\,\delta t \end{cases}$$

$$\bar{\kappa} \equiv \frac{\kappa_1 + \kappa_2}{2}$$

* Delov V.I., Sadchikov V.V., VANT (Mathematical Modeling of Physical Processes), 1, pp. 57–70 (2005) (in Russian).

§ Goncharov, E.A., Yanilkin, Yu., VANT (Mathematical Modeling of Physical Processes), 3, pp. 16–30 (2004) (in Russian).

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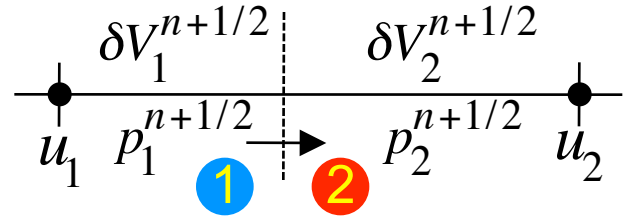
The mixed-cell predictor is built upon these relations.



- Based on these expressions, we update the individual volume fractions in the mixed cell:

$$\delta V_1^{n+1/2} = \beta_1 \, \delta V^{n+1/2} + \tfrac{1}{2}(\Delta p_{1,2}^n / \bar{\kappa}^n)\,(\delta t/2)$$

$$\delta V_2^{n+1/2} = \beta_2 \, \delta V^{n+1/2} - \tfrac{1}{2}(\Delta p_{1,2}^n / \bar{\kappa}^n)\,(\delta t/2)$$

$p_1^n - p_2^n$

$\frac{1}{2}(\rho_1^n c_{s,1}^n + \rho_2^n c_{s,2}^n)$

where β_k obey: $\beta_1 + \beta_2 = 1$, $\beta_k \geq 0$ (like the volume fraction)

- We update the individual materials' pressures:

$$p_k^{n+1/2} = p_k^n - \left((c_{s,k}^n)^2 / \tau_k^n\right)\left(\delta V_k^{n+1/2} / V_k^n\right)$$

Adiabatic update

- We postulate the corresponding overall mixed-cell pressure:

$$p_{i_{\text{mix}}+1/2}^{n+1/2} = \sum_k \theta_k \, p_k^{n+1/2} \quad , \quad \theta_1 + \theta_2 = 1 \, , \quad \theta_k \geq 0$$

We set: $\theta_k = \beta_k = f_k$

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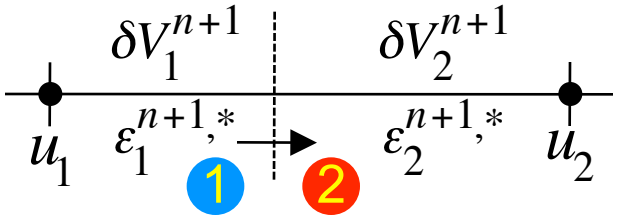
The mixed-cell corrector requires further assumptions.



- Using the results of the previous page, we update several mixed-cell quantities for each material, including the SIE:

$$\varepsilon_1^{n+1,*} = \varepsilon_1^n - \beta_1^{n+1/2} p_1^{n+1/2} \delta V_1^{n+1} \big/ M_1 - \tfrac{1}{2} p_1^{n+1/2} (\Delta p_{1,2}^{n+1/2} \big/ \bar{\kappa}^{n+1/2}) (\delta t \big/ M_1)$$

$$\varepsilon_2^{n+1,*} = \varepsilon_2^n - \beta_2^{n+1/2} p_2^{n+1/2} \delta V_2^{n+1} \big/ M_2 + \tfrac{1}{2} p_2^{n+1/2} (\Delta p_{1,2}^{n+1/2} \big/ \bar{\kappa}^{n+1/2}) (\delta t \big/ M_2)$$

- There is a problem: this SIE update is *not consistent* with the total work done on the cell, i.e.,

$$\sum_k M_k \, d\varepsilon_k^{n+1,*} \neq -p_{i_{\text{mix}}+1/2}^{n+1/2} \, d V_{i_{\text{mix}}+1/2}^{n+1}$$

- This implies total energy is not conserved: not good!
- Can we re-distribute energy to ensure consistency?

Answer: *Yes* — and one approach is given on the next slides…

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We need equations to distribute the internal energy "discrepancy" and ensure balance.

- Let $d\tilde{\varepsilon}_k$ be the change in SIE that guarantees consistency:

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

- One can show the *total* internal energy discrepancy is:

$$d\mathcal{E}^{n+1/2} \equiv \sum_k M_k \boxed{d\tilde{\varepsilon}_k} = \boxed{\frac{(p_1^{n+1/2} - p_2^{n+1/2})^2}{\kappa_1^{n+1/2} + \kappa_2^{n+1/2}} \delta t} \qquad \text{Ⓐ}$$

- There is a pressure pressure change due to $d\tilde{\varepsilon}_k$ — assume it:
  - (i) is the same for both materials, and
  - (ii) depends *only* on the energy (and *not* on the density):

$$\Rightarrow \boxed{d\tilde{P}} = \left(\partial p_1 / \partial \varepsilon_1\right)\Big|_{\rho_1} d\tilde{\varepsilon}_1 \quad \text{and} \quad \boxed{d\tilde{P}} = \left(\partial p_2 / \partial \varepsilon_2\right)\Big|_{\rho_2} d\tilde{\varepsilon}_2 \qquad \text{Ⓑ}$$

- We can solve the system of equations given by Ⓐ & Ⓑ

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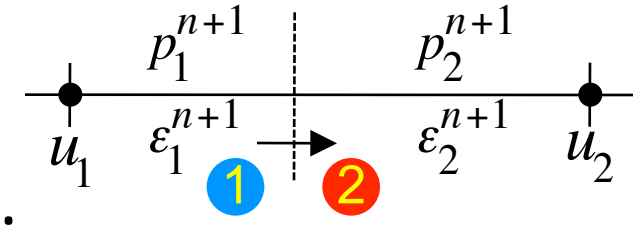
We obtain solutions to these equations using the other updated values.



- Combining Ⓐ and Ⓑ from the previous page, one obtains:

$$d\tilde{P} = \frac{\boxed{d\varepsilon^{n+1/2}}}{[m_1/(\partial p_1/\partial \varepsilon_1)_{\rho_1}^{n+1}] + [m_2/(\partial p_2/\partial \varepsilon_2)_{\rho_2}^{n+1}]}$$

- Evaluate the thermodynamic derivatives:

$$\left(\partial p_k/\partial \varepsilon_k\right)_{\rho_k}^{n+1} \approx \boxed{\left.\left(\frac{\partial p_k}{\partial \varepsilon_k}\right)\right|_{\rho_k}\left(\rho_k^{n+1}, \varepsilon_k^{n+1,*}\right)}$$

- Compute $d\tilde{P}$ and use that value to calculate $d\tilde{\varepsilon}_1$ and $d\tilde{\varepsilon}_2$:

$$d\tilde{\varepsilon}_1 = d\tilde{P}\Big/\left(\partial p_1/\partial \varepsilon_1\right)_{\rho_1} \quad \text{and} \quad d\tilde{\varepsilon}_2 = d\tilde{P}\Big/\left(\partial p_2/\partial \varepsilon_2\right)_{\rho_2}$$

- Correct the SIEs and update the pressures:

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

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We compare results of this method (KSR) with three other approaches.

- Pure Material:
  - Use the basic predictor-corrector method with no mixed cell.
  - Straightforward algorithm for an idealized problem.
  - (+) No mixed cell assumptions.
  - (−) No mixed cell assumptions.
- Kamm & Shashkov* (KS):
  - Solve a local Riemann problem in the mixed cell.
  - Use that to find "optimal" states of each material.
  - (+) Physics-based, good-quality solutions.
  - (−) More complicated, difficult to extend to 2D & material strength.
- Tipton§:
  - Add relaxation term to each pressures, so that they are all equal.
  - Exactly solve the resulting equations for the relaxation pressure.
  - (+) Robust, fast, widely used, extended to multi-D & material strength.
  - (−) Rough-and-ready assumptions, fair solutions.

* Kamm, J., Shashkov, M., *Comm. Comput. Phys.*, **7**, pp. 927–976 (2010).

§ Shashkov, M., *Int. J. Numer. Meth. Fluids*, **56**, pp. 1497–1504 (2007).

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Kamm & Shashkov (KS) break the pressure equilibration assumption of Després* using the solution to a local Riemann problem.

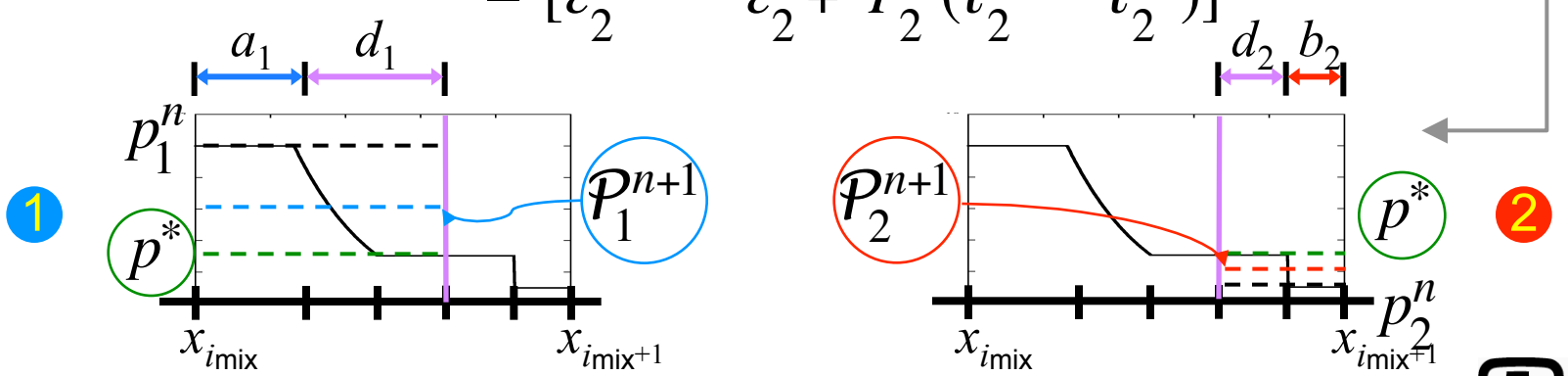
- Pressure relaxation in the mixed cell reduces to the solution of a minimization problem in τ_1^{n+1}, ε_1^{n+1}, τ_2^{n+1}, ε_2^{n+1}

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

subject to:

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

Mixed-cell Riemann Problem



*Després, B., Lagoutière, F., *Prog. Comput. Fluid Dyn.* **7**, pp. 295–310 (2007).

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

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

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

Unknown

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

Unknown

Predictor pressure of k-th material

$$p_k^{n+1/2} + \boxed{R_k} = \boxed{\hat{p}^{n+1/2}}$$

Overall predictor pressure

where $\boxed{R_k} = -\left(cs_k^n \big/ \tau_k^n\right)\left(L^n \big/ \delta t\right)\left(\boxed{\delta V_k^{n+1/2}} \Big/ V_k^n\right)$

Relaxation term for k-th material

- *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 $\hat{p}^{n+1/2}$ and $\delta V_k^{n+1/2}$ in closed form.
- The second step of a two-step time-integrator uses this information to obtain the final updated values.

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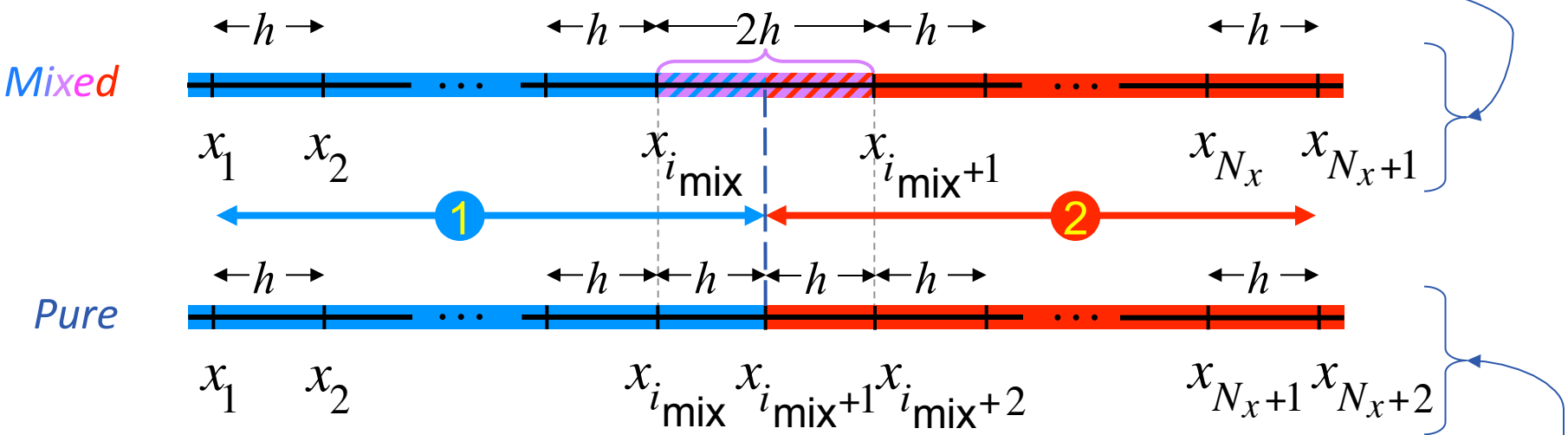
We examine the results of this method on standard test problems.

- The test problems were run similarly:
  - N_x zones on $x_{\text{min}} \le x < x_{\text{max}}$ 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
- Graphical results for the test problems include:
  - "Snapshots": fixed-in-*time*, *spatial* solution, on the *whole mesh*
  - "Histories": fixed-in-*space*, *temporal* solution, *in the mixed cell*

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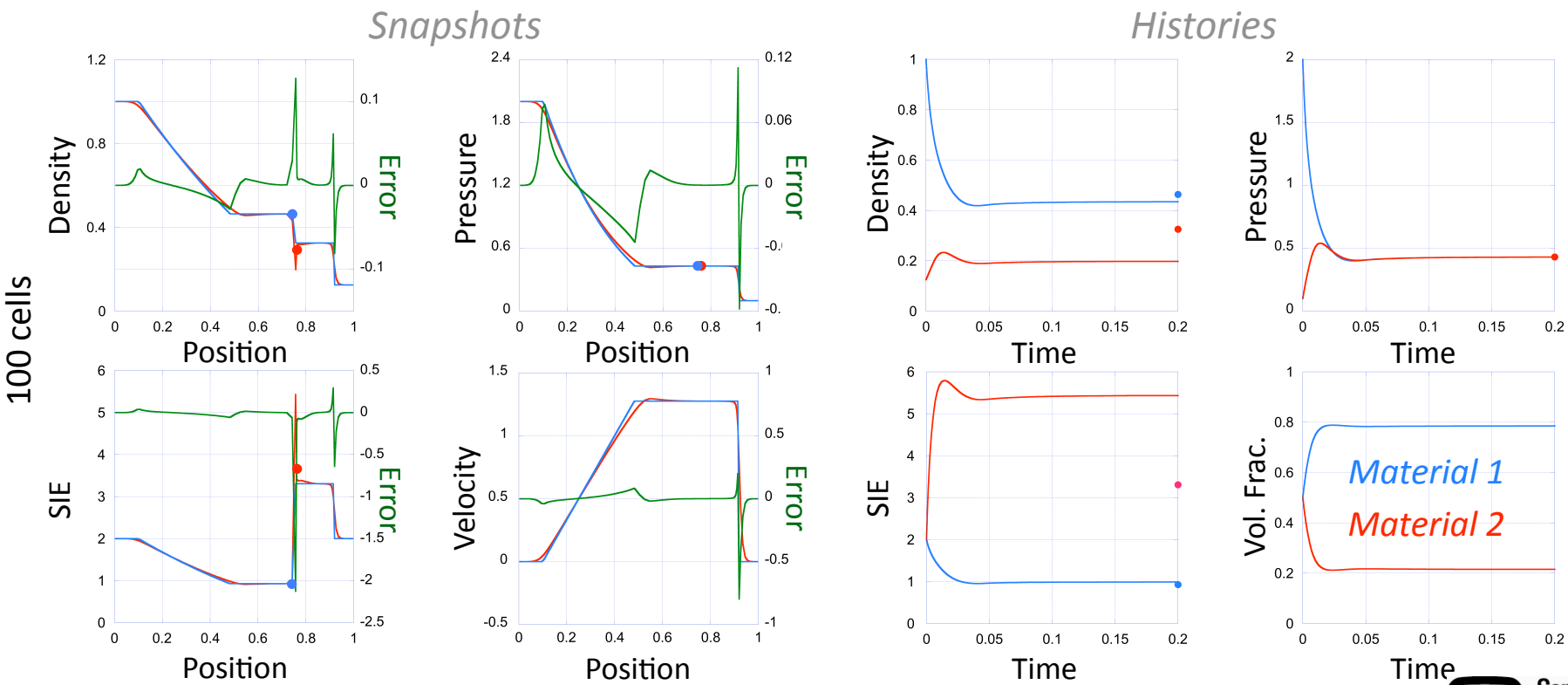
The results for the modified Sod shock tube indicate that this approach is reasonable.

- Modified Sod problem initial conditions:

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



"Closed-form" – *Computed* = *Error*

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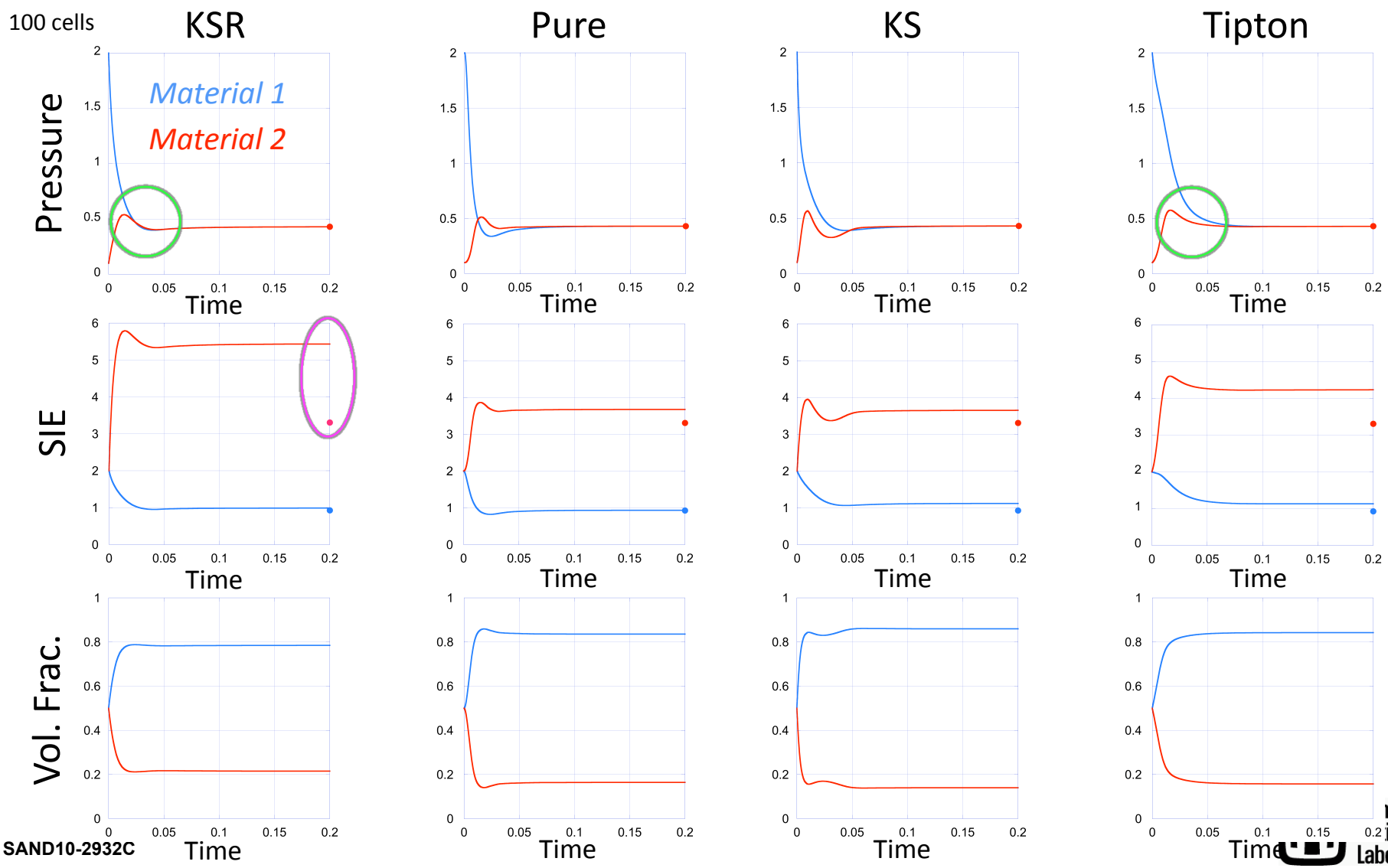
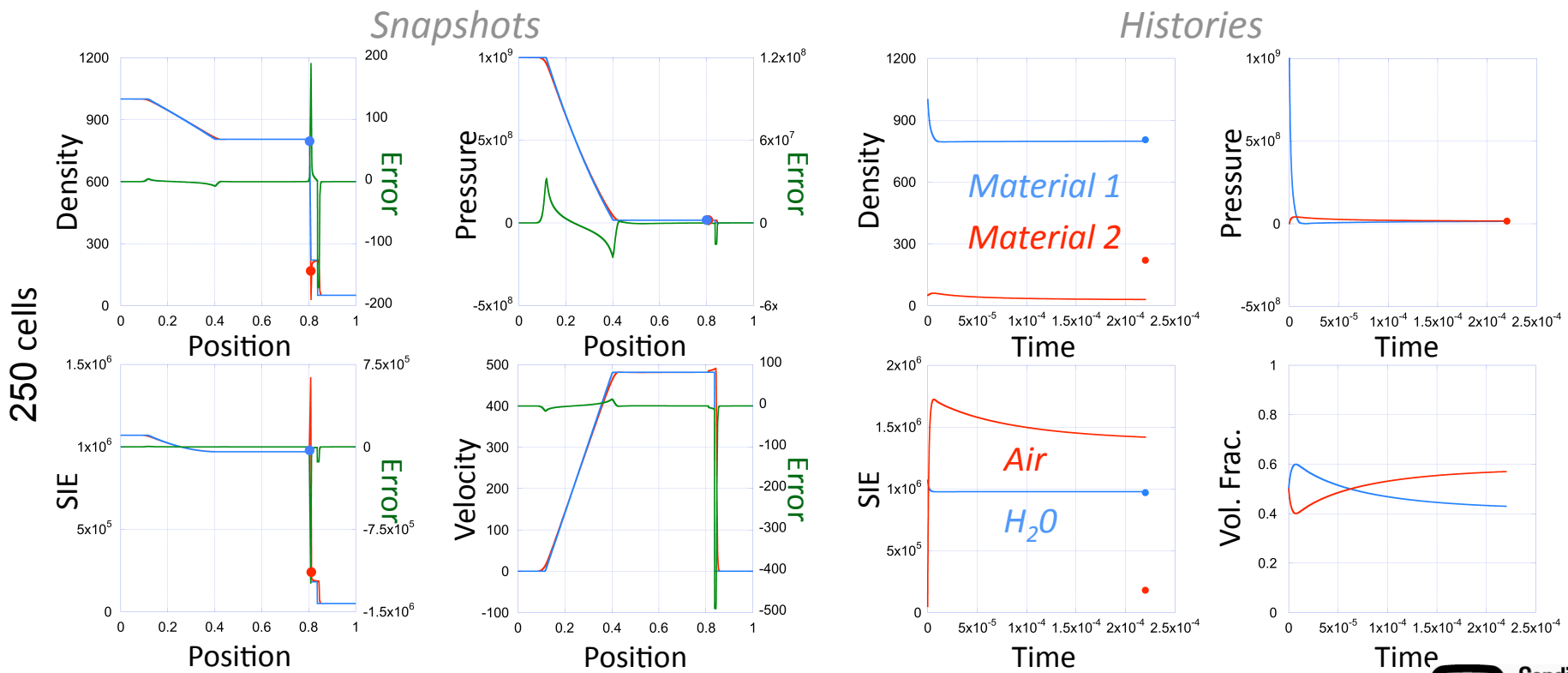
Mixed cell histories for the modified Sod problem exhibit some differences among the various methods.



A water-air shock tube* is a *de facto* standard test for multimaterial hydro solvers.

- Water-air shock tube initial conditions:

$$(\rho,p,u,\gamma,p_\infty) = \begin{cases} (1.e+3,1.e+9,0.0,4.4,6.e+8), & 0\le x<0.7 \\ (5.e+1,1.e+6,0.0,1.4,0.0), & 0.7<x\le 1.0 \end{cases} \qquad p = (\gamma-1)\rho e - \gamma p_\infty \qquad t_{\text{final}} = 2.2e\text{-}4$$



"Closed-form" – *Computed* = *Error*

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

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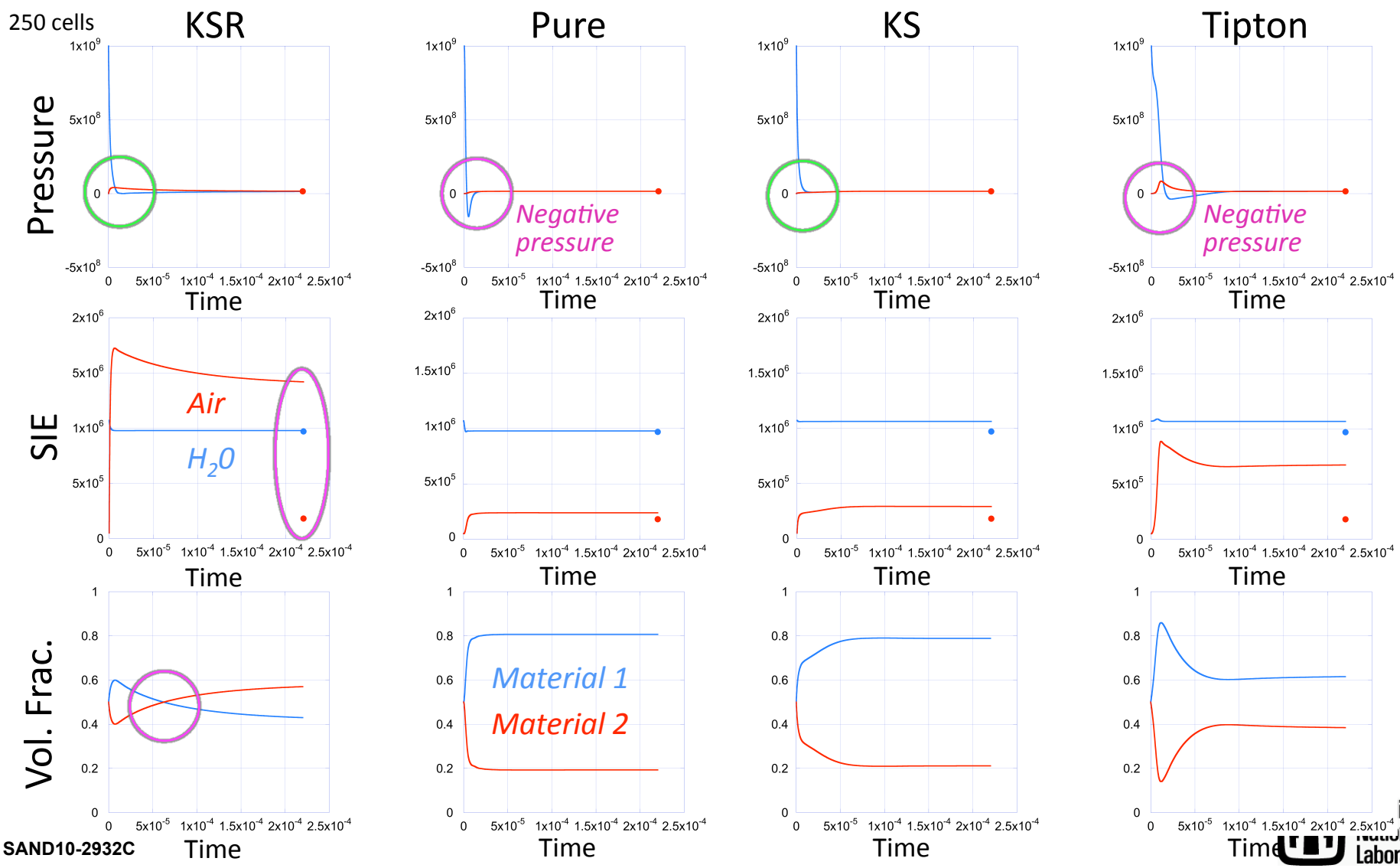
The KSR approach on the water-air shock tube has both good and bad qualities.



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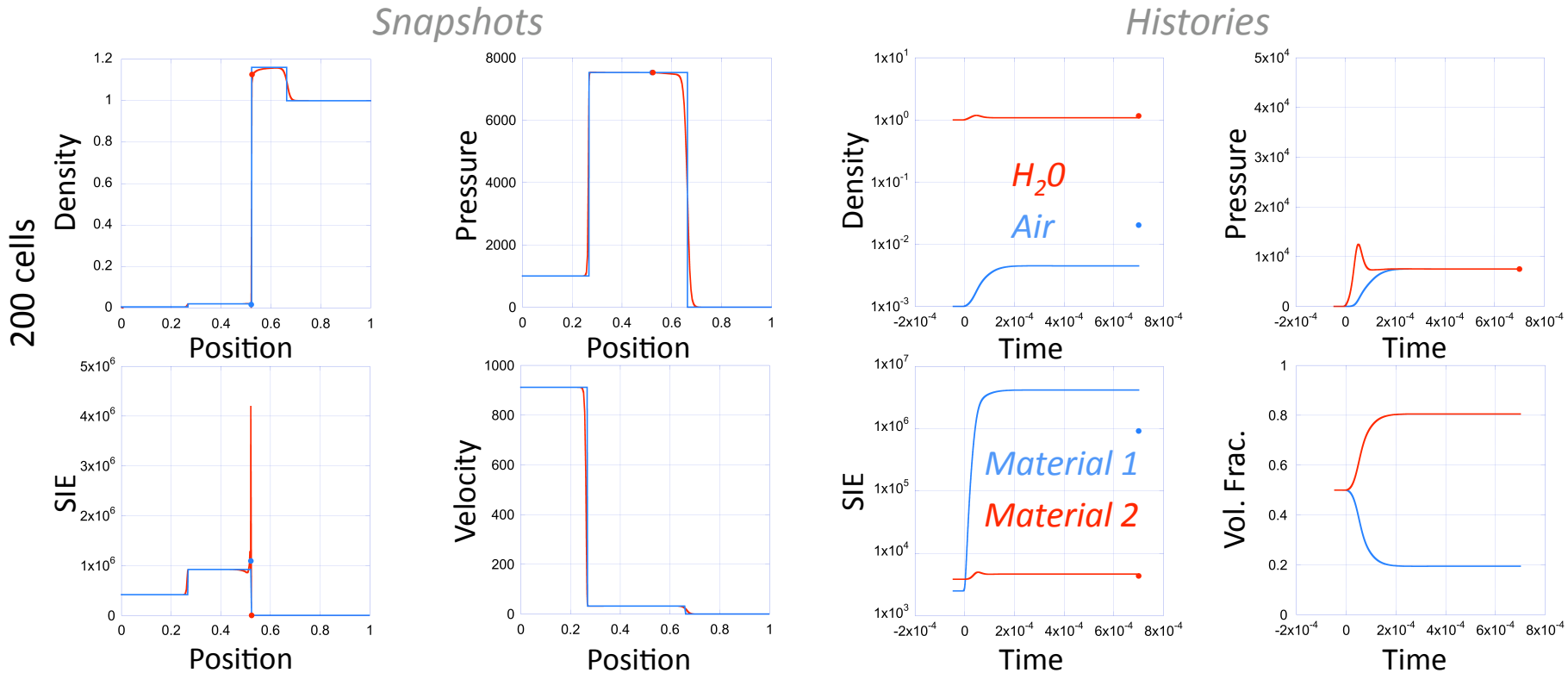
A shock problem of Wang et al.* is more challenging and highlights "features" of these models.

$$(\rho,p,u,\gamma,p_\infty)=\begin{cases}(5.96\text{e-}3,\ 1.0\text{e+}3,\ 9.12\text{e+}2,\ 1.4,\ 0\ ), & 0<x<0.45\\ (1.0\text{e-}3,\ 1.0,\ 0,\ 1.4,\ 0\ ), & 0.45<x<0.5\\ (1.0,\ 1.0,\ 0,\ 7.15,\ 3.31\text{e+}3), & 0.5<x<1\end{cases}$$

$Ma \approx 29$

t_{init} = -4.56e-5

t_{final} = 7.0e-4



"Closed-form" *Computed*

* C.W. Wang et al. "A real ghost fluid method for the simulation of multi-medium compressible flow," *SIAM J. Sci.. Comput.* **28**, 278–302 (2006).

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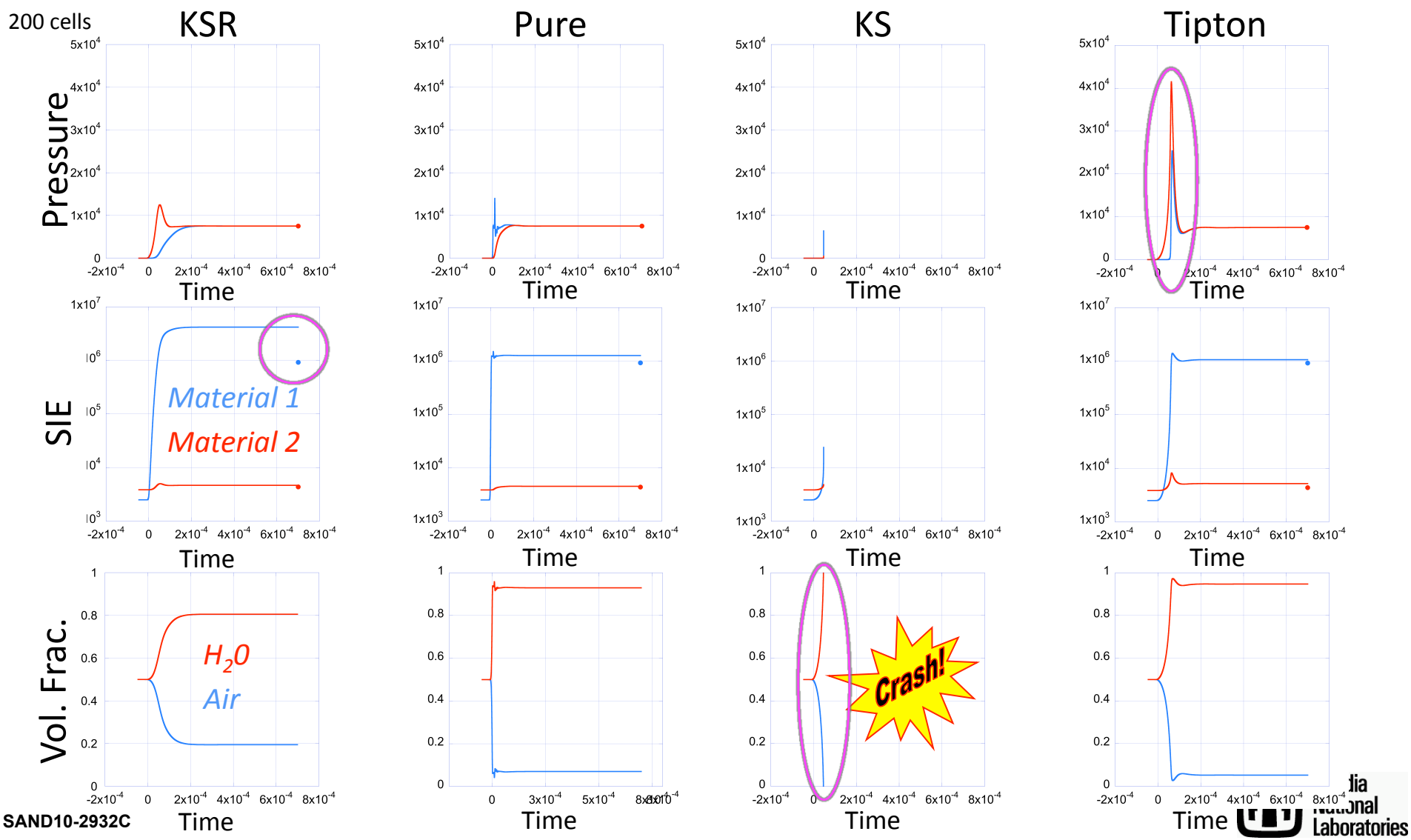
The KSR approach on the Wang et al. shock tube has both good and bad qualities.



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Summary, conclusions, and future work…

- The mixed-cell problem for Lagrangian hydrodynamics remains open.
- A model inspired by Delov & Sadchikov and Goncharov & Yanilkin:
  - Uses a linearized Riemann solver for the interface velocity
  - *Predicts* the SIE with a simple but non-conservative model
  - *Corrects* the SIE to ensure that the updated $p\,dV$ work is consistent
  - Ensures that the final thermodynamic state is consistent
- This model has plusses and minuses:
  - (+) Fast, simple, good-quality solutions
  - (•) Extension to 2D requires pair-wise, directional interactions: Harrison et al.*
  - (−) "Funny" SIE; strength: not obvious, but (hopefully) do-able
- Rigorous evaluation against different methods on test problems:
  - Both qualitative and quantitative evaluation is necessary
  - We must conduct more tests (small volume fractions)
- Extend this method to account, e.g., for material strength and voids.

* See also: Kamm, J., Shashkov, M., Fung, J., Harrison, A., Canfield, T., *Int. J. Numer. Meth. Fluids.*, in press (2010).

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