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A Single-Pressure Closure Model for 1-D Lagrangian Hydrodynamics Based on the Riemann Problem

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A physics-inspired model closes a two-material, single-pressure, mixed-cell hydro model.

- 1-D hydrodynamics is a building-block for higher-dimensional methods:
  - Allows the careful investigation of basic assumptions.
  - Highlights the details and the features of a particular method.
- Two-material, single-pressure models are a basic element of multi-material hydrodynamics:
  - Homogenize materials via single-velocity, single-pressure model.
  - Sub-cell interaction assumptions appear in the model equations.
- Models for a *gradual* (as opposed to *instantaneous*) approach to pressure equilibrium may be closer to the underlying physics.
  - Simplified models capture the essence of the relevant physics.
- A Riemann-problem-inspired approach demonstrates some promising characteristics on various test problems.
  - Results are quantified against exact solutions.
  - Mixed-cell properties are evaluated and quantified.

Outline of this presentation

- **1-D, 2-material Lagrangian hydrodynamics**: the closure problem for mixed cells.
- **Instantaneous pressure equilibration**: this assumption gives closed-form solutions for polytropic gases.
- **Pressure relaxation model**: the physics, mathematics, and numerics of a local Riemann problem.
- **Implementation**: how to use this model with a predictor-corrector scheme.
- **Test problem results**: Sod shock tube, a shock-contact problem, the water-air shock tube + comparison with other methods.
- **Summary**: Conclusions + future work.

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

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

Mass: $$\rho^0 \frac{\partial \tau}{\partial t} - \frac{\partial u}{\partial x} = 0 \qquad \tau \equiv 1/\rho$$

Momentum: $$\rho^0 \frac{\partial u}{\partial t} + \frac{\partial P}{\partial x} = 0 \qquad \rho^0 = \rho^0(x) \equiv \rho(x,t=0)$$

Energy: $$\rho^0 \frac{\partial e}{\partial t} + \frac{\partial}{\partial x}(Pu) = 0 \qquad e \equiv \varepsilon + (1/2)\,u^2$$

Thermodynamics: $$P = \mathcal{P}(\varepsilon,\tau)$$

Specific Internal Energy (SIE)

- With the 1-D equations, we can:
  - Impose design principles clearly
  - Test fundamental algorithms
  - Quantitatively evaluate algorithm performance

This model is for a two-material, single-pressure cell with *instantaneous* equilibration.

- The four-equation model for the mixed cell is:

Assign Spec. Vol.: $c_1\,\tau_1^{n+1} + c_2\,\tau_2^{n+1} = \tau^{n+1}$

Assign SIE: $c_1\,\varepsilon_1^{n+1} + c_2\,\varepsilon_2^{n+1} = \varepsilon^{n+1}$

Mass fractions: $c_k \equiv m_k / m_{\text{mixed}} \rightarrow \text{fixed},\ \forall\, t$

Equality of Pressure:

$$\begin{cases} \mathcal{P}_1(\varepsilon_1^{n+1}, \tau_1^{n+1}) = \mathcal{P}_2(\varepsilon_2^{n+1}, \tau_2^{n+1}) \\ \text{i.e.,} \quad p_1^{n+1} = p_2^{n+1} \end{cases}$$

Pressure equilibration over Δt

Equality of Change in Heat: $\varepsilon_1^{n+1} - \varepsilon_1^n + P_1(\tau_1^{n+1} - \tau_1^n) = \varepsilon_2^{n+1} - \varepsilon_2^n + P_2(\tau_2^{n+1} - \tau_2^n)$

- In the last equation, one must make a modeling choice for the expressions P_1 and P_2 in terms of τ_k^n, ε_k^n, τ_k^{n+1}, ε_k^{n+1}
  - Why? Because this (equilibrium) thermodynamics statement ($dQ_1 = dQ_2$) occurs over the (discrete) timestep, $\Delta t \equiv t^{n+1} - t^n$

Three obvious choices for the pressure in the equality-of-heat-change equation:

- Model #1: Fully Explicit (*FE*), with $P_1 \equiv p_1^n$ and $P_2 \equiv p_2^n$

$$\Rightarrow \quad \varepsilon_1^{n+1} - \varepsilon_1^n + p_1^n (\tau_1^{n+1} - \tau_1^n) = \varepsilon_2^{n+1} - \varepsilon_2^n + p_2^n (\tau_2^{n+1} - \tau_2^n)$$

- Model #2: Fully Implicit (*FI*), with $P_1 \equiv p_1^{n+1}$ and $P_2 \equiv p_2^{n+1}$

$$\Rightarrow \quad \varepsilon_1^{n+1} - \varepsilon_1^n + p_1^{n+1} (\tau_1^{n+1} - \tau_1^n) = \varepsilon_2^{n+1} - \varepsilon_2^n + p_2^{n+1} (\tau_2^{n+1} - \tau_2^n)$$

- Model #3: "Thermodynamically Consistent" (*TC*), with

$$P_1 \equiv \tfrac{1}{2}(p_1^n + p_1^{n+1}) \quad \text{and} \quad P_2 \equiv \tfrac{1}{2}(p_2^n + p_2^{n+1})$$

$$\Rightarrow \quad \varepsilon_1^{n+1} - \varepsilon_1^n + \tfrac{1}{2}(p_1^n + p_1^{n+1})(\tau_1^{n+1} - \tau_1^n) = \varepsilon_2^{n+1} - \varepsilon_2^n + \tfrac{1}{2}(p_2^n + p_2^{n+1})(\tau_2^{n+1} - \tau_2^n)$$

For polytropic gases, there are closed-form sol'ns to the closure equations in each case.

- Fully Implicit case (#2):

$$\varepsilon_1^{n+1} - \varepsilon_1^n + p_1^{n+1}(\tau_1^{n+1} - \tau_1^n) = \varepsilon_2^{n+1} - \varepsilon_2^n + p_2^{n+1}(\tau_2^{n+1} - \tau_2^n)$$

- Obtained by Loubère, Shashkov, Després & Lagoutière:

$$p = \frac{c_1 c_2(\gamma_1 - \gamma_2)(\varepsilon_1^n - \varepsilon_2^n) + [c_1\gamma_2(\gamma_1 - 1) + c_2\gamma_1(\gamma_2 - 1)]\,\varepsilon^{n+1}}{(c_2\gamma_1 + c_1\gamma_2)\tau^{n+1} - c_1 c_2(\gamma_1 - \gamma_2)(\tau_1^n - \tau_2^n)}$$

$$\varepsilon_1^{n+1} = \frac{\gamma_2\varepsilon^{n+1}\tau^{n+1} + c_2[(\gamma_2 - 1)\varepsilon^{n+1}(\tau_1^n - \tau_2^n) + (\varepsilon_1^n - \varepsilon_2^n)\tau^{n+1}]}{(c_2\gamma_1 + c_1\gamma_2)\tau^{n+1} - c_1 c_2(\gamma_1 - \gamma_2)(\tau_1^n - \tau_2^n)}$$

$$\tau_1^{n+1} = (\gamma_1 - 1)\,\frac{\gamma_2\varepsilon^{n+1}\tau^{n+1} + c_2[(\gamma_2 - 1)\varepsilon^{n+1}(\tau_1^n - \tau_2^n) + (\varepsilon_1^n - \varepsilon_2^n)\tau^{n+1}]}{[c_1\gamma_2(\gamma_1 - 1) + c_2\gamma_1(\gamma_2 - 1)]\,\varepsilon^{n+1} + c_1 c_2(\gamma_1 - \gamma_2)(\varepsilon_1^n - \varepsilon_2^n)}$$

Valid $\forall\ \gamma_1, \gamma_2$

  - Similar results for ε_2^{n+1} and τ_2^{n+1}

- Fully Explicit (#1) , Thermo. Consist. (#3) are complicated…

There are two solutions for the Fully Explicit case.

- Fully Explicit case (#1):

$$\varepsilon_1^{n+1} - \varepsilon_1^n + p_1^n(\tau_1^{n+1} - \tau_1^n) = \varepsilon_2^{n+1} - \varepsilon_2^n + p_2^n(\tau_2^{n+1} - \tau_2^n)$$

- First solution for p:

$$\begin{aligned} p = {} & [2(c_1+c_2)\tau^{n+1}]^{-1}\{\varepsilon^{n+1}[c_1(\gamma_1-1)+c_2(\gamma_2-1)] \\ & -\tau^{n+1}[c_2(\gamma_1-1)p_1^n + c_1(\gamma_2-1)p_2^n] \\ & +c_1c_2(\gamma_1-\gamma_2)(\varepsilon_1^n - \varepsilon_2^n + p_1^n\tau_1^n - p_2^n\tau_2^n) \\ & -[-4c_2(\gamma_1-\gamma_2)(\gamma_2-1)(c_2p_1^n + c_1p_2^n)\tau^{n+1} \\ & \times[c_1(\varepsilon_1^n - \varepsilon_2^n + p_1^n\tau_1^n - p_2^n\tau_2^n) - \varepsilon^{n+1} - p_1^n\tau^{n+1}] \\ & +\{\varepsilon^{n+1}[c_1(1-\gamma_1)+c_2(1-\gamma_2)] \\ & +\tau^{n+1}(1-\gamma_2)(c_1p_2^n + c_2p_1^n) \\ & +c_2(\gamma_1-\gamma_2)[p_1^n\tau_1^n - c_1(\varepsilon_1^n - \varepsilon_2^n + p_1^n\tau_1^n - p_2^n\tau_2^n)]\}^2]^{1/2}\} \end{aligned}$$

- Second solution for p:

$$\begin{aligned} p = {} & [2(c_1+c_2)\tau^{n+1}]^{-1}\{\varepsilon^{n+1}[c_1(\gamma_1-1)+c_2(\gamma_2-1)] \\ & +\tau^{n+1}[c_2(\gamma_1-1)p_1^n + c_1(\gamma_2-1)p_2^n] \\ & +c_1c_2(\gamma_1-\gamma_2)(\varepsilon_1^n - \varepsilon_2^n + p_1^n\tau_1^n - p_2^n\tau_2^n) \\ & +[-4c_2(\gamma_1-\gamma_2)(\gamma_2-1)(c_2p_1^n + c_1p_2^n)\tau^{n+1} \\ & \times[c_1(\varepsilon_1^n - \varepsilon_2^n + p_1^n\tau_1^n - p_2^n\tau_2^n) - \varepsilon^{n+1} - p_1^n\tau^{n+1}] \\ & +\{\varepsilon^{n+1}[c_1(1-\gamma_1)+c_2(1-\gamma_2)] \\ & +\tau^{n+1}(1-\gamma_2)(c_2p_1^n + c_1p_2^n) \\ & +c_2(\gamma_1-\gamma_2)[p_1^n\tau_1^n - c_1(\varepsilon_1^n - \varepsilon_2^n + p_1^n\tau_1^n - p_2^n\tau_2^n)]\}^2]^{1/2}\} \end{aligned}$$

- As $\gamma_1 \to \gamma_2$, these solutions approach the same limit:

$$p = (\gamma - 1)\,\varepsilon^{n+1}/\tau^{n+1}$$

And two solutions in the "Thermo. Consist." case:

- Thermodynamically Consistent case (#3):

$$\varepsilon_1^{n+1} - \varepsilon_1^n + \boxed{\tfrac{1}{2}(p_1^n + p_1^{n+1})}(\tau_1^{n+1} - \tau_1^n) = \varepsilon_2^{n+1} - \varepsilon_2^n + \boxed{\tfrac{1}{2}(p_2^n + p_2^{n+1})}(\tau_2^{n+1} - \tau_2^n)$$

- First solution for p:

$$\begin{aligned}
p = \{&2c_1c_2(\gamma_1-\gamma_2)(\tau_1^n-\tau_2^n)\\
&-2[c_1(1+\gamma_2)+c_2(1+\gamma_1)]\tau^{n+1}\}^{-1}\\
\times\{&-\varepsilon^{n+1}[c_1(\gamma_1-1)(\gamma_2+1)+c_2(\gamma_1+1)(\gamma_2-1)]\\
&+\tau^{n+1}[c_2(\gamma_1-1)p_1^n+c_1(\gamma_2-1)p_2^n]\\
&-c_1c_2(\gamma_1-\gamma_2)(2\varepsilon_1^n-2\varepsilon_2^n+p_1^n\tau_1^n-p_2^n\tau_2^n)\\
&+[-4c_1c_2\varepsilon^{n+1}(\gamma_1-\gamma_2)(\gamma_1-1)(\gamma_2-1)\\
&\times(c_2p_1^n+c_1p_2^n)(\tau_1^n-t_2^n)\\
&+4[c_1(1+\gamma_2)+c_2(1+\gamma_1)]\varepsilon^{n+1}\\
&\times(\gamma_1-1)(\gamma_2-1)(c_2p_1^n+c_1p_2^n)\tau^{n+1}\\
&+\{\varepsilon^{n+1}[c_1(\gamma_1-1)(\gamma_2+1)+c_2(\gamma_1+1)(\gamma_2-1)]\\
&-\tau^{n+1}[c_2(\gamma_1-1)p_1^n+c_1(\gamma_2-1)p_2^n]\\
&+c_1c_2(\gamma_1-\gamma_2)(2\varepsilon_1^n-2\varepsilon_2^n+p_1^n\tau_1^n-p_2^n\tau_2^n)\}^2]^{1/2}\}
\end{aligned}$$

- Second solution for p:

$$\begin{aligned}
p = \{&2c_1c_2(\gamma_1-\gamma_2)(\tau_1^n-\tau_2^n)\\
&-2[c_1(1+\gamma_2)+c_2(1+\gamma_1)]\tau^{n+1}\}^{-1}\\
\times\{&-\varepsilon^{n+1}[c_1(\gamma_1-1)(\gamma_2+1)+c_2(\gamma_1+1)(\gamma_2-1)]\\
&+\tau^{n+1}[c_2(\gamma_1-1)p_1^n+c_1(\gamma_2-1)p_2^n\\
&-c_1c_2(\gamma_1-\gamma_2)(2\varepsilon_1^n-2\varepsilon_2^n+p_1^n\tau_1^n-p_2^n\tau_2^n)\\
&-[-4c_1c_2\varepsilon^{n+1}(\gamma_1-\gamma_2)(\gamma_1-1)(\gamma_2-1)\\
&\times(c_2p_1^n+c_1p_2^n)(\tau_1^n-t_2^n)\\
&+4[c_1(1+\gamma_2)+c_2(1+\gamma_1)]\varepsilon^{n+1}\\
&\times(\gamma_1-1)(\gamma_2-1)(c_2p_1^n+c_1p_2^n)\tau^{n+1}\\
&+\{\varepsilon^{n+1}[c_1(\gamma_1-1)(\gamma_2+1)+c_2(\gamma_1+1)(\gamma_2-1)]\\
&-\tau^{n+1}[c_2(\gamma_1-1)p_1^n+c_1(\gamma_2-1)p_2^n]\\
&+c_1c_2(\gamma_1-\gamma_2)(2\varepsilon_1^n-2\varepsilon_2^n+p_1^n\tau_1^n-p_2^n\tau_2^n)\}^2]^{1/2}\}
\end{aligned}$$

- Again, as $\gamma_1 \to \gamma_2$, these approach the same limit:

$$p = (\gamma - 1)\,\varepsilon^{n+1}/\tau^{n+1}$$

The expressions for the updated value of the SIE for the FE case are more complicated…

- First solution for ε_1^{n+1}:

$$\begin{aligned}\varepsilon_1^{n+1} &= [2c_1(c_1+c_2)(\gamma_1-\gamma_2)]^{-1}\\ &\times\{\varepsilon^{n+1}(1-\gamma_2)(c_1+c_2)\\ &-\tau^{n+1}[c_2(\gamma_1-1)p_1^n+c_1(\gamma_2-1)p_2^n]\\ &+c_1(\gamma_1-\gamma_2)[\varepsilon^{n+1}+c_2(\varepsilon_1^n-\varepsilon_2^n+p_1^n\tau_1^n-p_2^n\tau_2^n)]\\ &-[-4c_2(\gamma_1-\gamma_2)(\gamma_2-1)(c_2p_1^n+c_1p_2^n)\tau^{n+1}\\ &\times[c_1(\varepsilon_1^n-\varepsilon_2^n+p_1^n\tau_1^n-p_2^n\tau_2^n)-\varepsilon^{n+1}-p_1^n\tau^{n+1}]\\ &+\{\varepsilon^{n+1}[c_1(1-\gamma_1)+c_2(1-\gamma_2)]\\ &+\tau^{n+1}(1-\gamma_2)(c_1p_2^n+c_2p_1^n)\\ &+c_2(\gamma_1-\gamma_2)[p_1^n\tau_1^{n+1}\\ &-c_1(\varepsilon_1^n-\varepsilon_2^n+p_1^n\tau_1^n-p_2^n\tau_2^n)]\}^2]^{1/2}\}\end{aligned}$$

- Second solution for ε_1^{n+1}:

$$\begin{aligned}\varepsilon_1^{n+1} &= [2c_1(c_1+c_2)(\gamma_1-\gamma_2)]^{-1}\\ &\times\{\varepsilon^{n+1}(1-\gamma_2)(c_1+c_2)\\ &-\tau^{n+1}[c_2(\gamma_1-1)p_1^n+c_1(\gamma_2-1)p_2^n]\\ &+c_1(\gamma_1-\gamma_2)[\varepsilon^{n+1}+c_2(\varepsilon_1^n-\varepsilon_2^n+p_1^n\tau_1^n-p_2^n\tau_2^n)]\\ &+[-4c_2(\gamma_1-\gamma_2)(\gamma_2-1)(c_2p_1^n+c_1p_2^n)\tau^{n+1}\\ &\times[c_1(\varepsilon_1^n-\varepsilon_2^n+p_1^n\tau_1^n-p_2^n\tau_2^n)-\varepsilon^{n+1}-p_1^n\tau^{n+1}]\\ &+\{\varepsilon^{n+1}[c_1(1-\gamma_1)+c_2(1-\gamma_2)]\\ &+\tau^{n+1}(1-\gamma_2)(c_1p_2^n+c_2p_1^n)\\ &+c_2(\gamma_1-\gamma_2)[p_1^n\tau_1^{n+1}\\ &-c_1(\varepsilon_1^n-\varepsilon_2^n+p_1^n\tau_1^n-p_2^n\tau_2^n)]\}^2]^{1/2}\}\end{aligned}$$

- What happens to these two solutions as $\gamma_1 \to \gamma_2$?

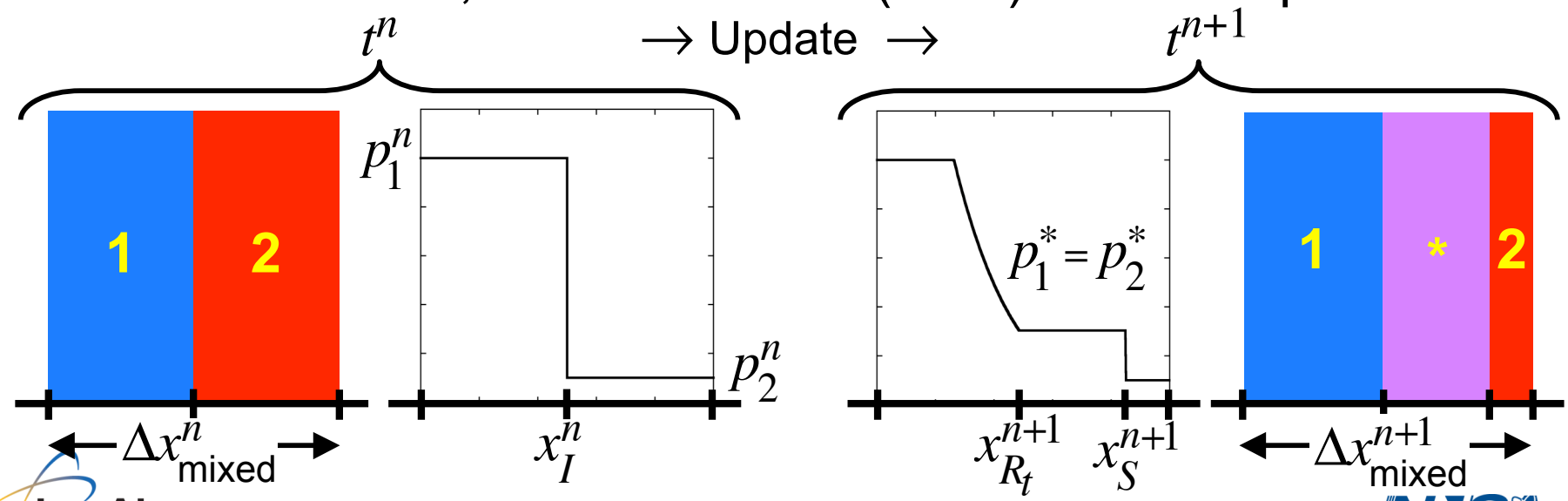
Full equations with $\gamma_1 = \gamma_2 = \gamma$ $\Rightarrow$

$$\varepsilon_1^{n+1} = \frac{[\varepsilon^{n+1}+p_2^n\tau^{n+1}+c_2(\varepsilon_1^n-\varepsilon_2^n+p_1^n\tau_1^n-p_2^n\tau_2^n)]}{(c_1+c_2)\varepsilon^{n+1}+(c_1p_2^n+c_2p_1^n)\tau^{n+1}}\,\varepsilon^{n+1}$$

- Analysis *suggests* a (removable) singularity in one sol'n.
  - Analysis incomplete…
  - Suggestive numerical evidence…
- TC case has more complicated expressions.

Instantaneous pressure equilibration is not consistent with the sub-grid-scale physics.

- Physical relaxation processes slow pressure equilibration.
  - We want to include this effect—but not the full physics.
  - Why not? Complicated, many unknown parameters.
- Instead, use the previous set of closure relations…
  - …but modify the "instantaneous" pressure-equilibration.
- How? A physics-inspired approach à la Godunov: use the 2-material, mixed cell as a (local) Riemann problem.



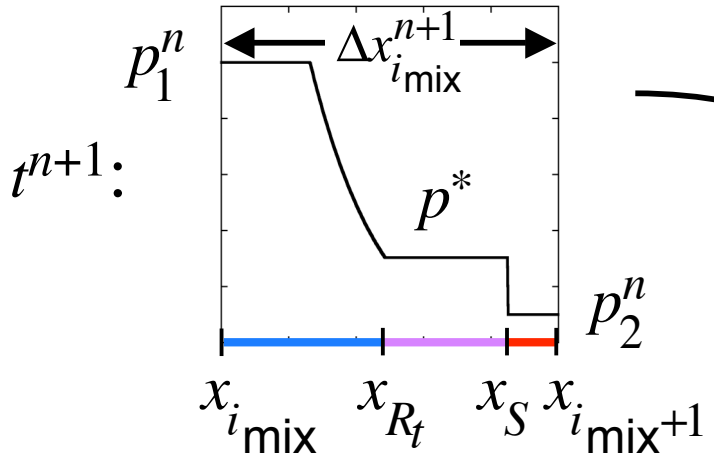
We can work out the details of the Riemann-problem-based pressure expressions.

- The initial (start-of-timestep) material interface is:

$$x_{\text{interface}} = x_{i_{\text{mix}}} + f_1 (x_{i_{\text{mix}+1}} - x_{i_{\text{mix}}})$$

f_1: Volume Fraction Material 1

- For either polytropic gas or stiffened-gas EOS, there are exact expressions for the Riemann wave speeds*
  - For general EOS, these can be approximated…
- With these wave speeds, a simple geometrical average for the (single) overall cell pressure can be derived:



$$\beta_1 = (x_{R_t} - x_{i_{\text{mix}}}) \Big/ \Delta x_{i_{\text{mix}}}^{n+1}$$

$$\beta_2 = (x_S - x_{R_t}) \Big/ \Delta x_{i_{\text{mix}}}^{n+1}$$

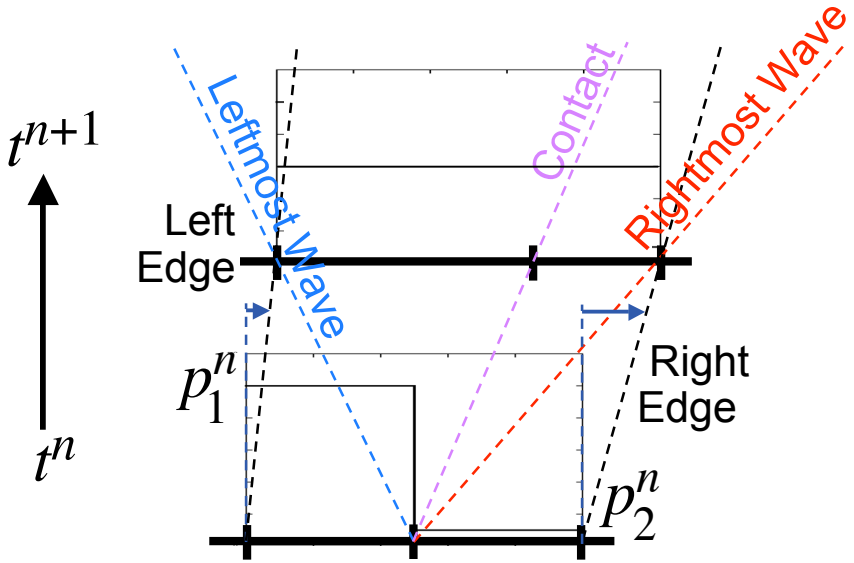
$$\beta_3 = (x_{i_{\text{mix}+1}} - x_S) \Big/ \Delta x_{i_{\text{mix}}}^{n+1}$$

$$\Rightarrow p_{i_{\text{mix}}}^{n+1} = \beta_1 p_1^n + \beta_2 p^* + \beta_3 p_2^n$$

*Gottlieb, J.J., and Groth, C.P.T., *J. Comp. Phys.* **78**, pp. 437–458 (1988); Plohr, B.,*AIAA J.* **26**, pp. 470–478 (1988).

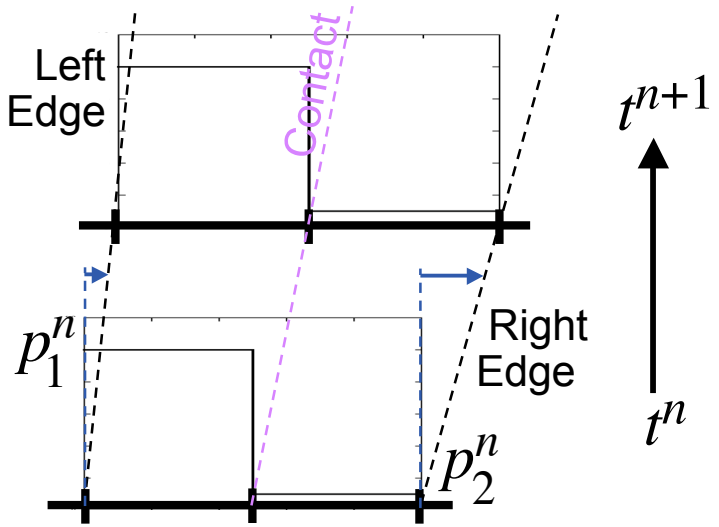
With this approach, a pressure-relaxation equation must satisfy two limiting cases.

- *Perfect equilibration* in Δt:



$$\mathcal{P}_1(\varepsilon_1^{n+1},\tau_1^{n+1}) = p^*$$
$$\mathcal{P}_2(\varepsilon_2^{n+1},\tau_2^{n+1}) = p^*$$

- *Pressure unchanged* in Δt:



$$\mathcal{P}_1(\varepsilon_1^{n+1},\tau_1^{n+1}) = p_1^n$$
$$\mathcal{P}_2(\varepsilon_2^{n+1},\tau_2^{n+1}) = p_2^n$$

- The pressure relaxation scheme should satisfy these limits.

This pressure-relaxation equation includes a modification from the local Riemann solution.

- Relax the pressure according to the following relation:

$$\delta p \equiv a_1\left[\mathcal{P}_1(\varepsilon_1^{n+1},\tau_1^{n+1})-p_1^n\right]+d_1\left[\mathcal{P}_1(\varepsilon_1^{n+1},\tau_1^{n+1})-p^*\right] - b_2\left[\mathcal{P}_2(\varepsilon_2^{n+1},\tau_2^{n+1})-p_2^n\right]-d_2\left[\mathcal{P}_2(\varepsilon_2^{n+1},\tau_2^{n+1})-p^*\right]=0$$

- The parameters a_1, d_1, d_2, b_2 are non-dimensional measures of the extent of the wave propagation:

p_1^n { a_1= |(left edge) - (leftmost wave)|/Δx^{n+1}

p^* { d_1= |(leftmost wave) - (contact)|/Δx^{n+1}

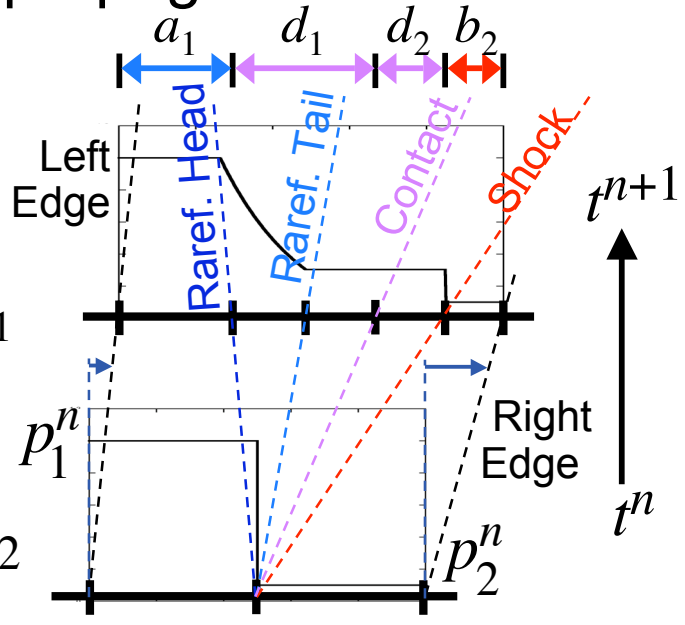
d_2= |(contact) - (rightmost wave)|/Δx^{n+1}

p_2^n { b_2= |(rightmost wave) - (right edge)|/Δx^{n+1}

(i) $a_1=b_2=0 \Rightarrow \mathcal{P}_1=\mathcal{P}_2=p^*, \forall\, d_1,d_2$

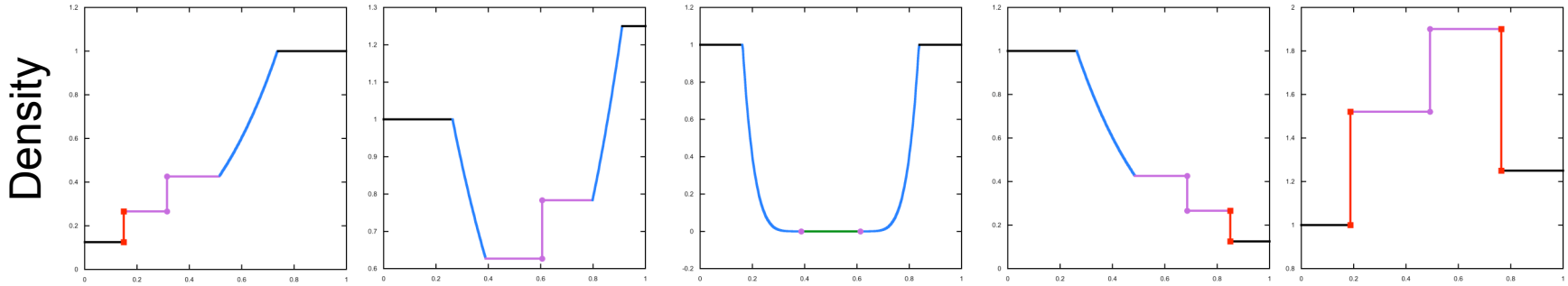
(ii) $d_1=d_2=0 \Rightarrow \mathcal{P}_1=p_1^n \wedge \mathcal{P}_2=p_2^n, \forall\, a_1,a_2$

(iii) By construction $a_1 + d_1 + d_2 + b_2 = 1$



This approach generalizes to all possible Riemann-problem solution states.

- For example, the polytropic gas Riemann problem has five fundamentally different solutions:



SCR RCR RCVCR RCS SCS

R=Rarefaction C=Contact V=Vacuum S=Shock

- In each case, the leading right-going and left-going waves and their wave speeds can be determined.
- These wave speeds can be used to obtain values for (i) the relaxation equation and (ii) the overall cell pressure model, each in terms of the mat'l-1, *-state, and mat'l-2 pressures.

These four-equation models can be solved with Newton's method for any EOS.

- We assume that the necessary thermodynamic derivatives of the pressure are available from the EOS.
- The four equations in the four unknowns, ε_1^{n+1}, τ_1^{n+1}, ε_2^{n+1}, τ_2^{n+1}, become:

$$f_1 \equiv c_1\ \tau_1^{n+1} + c_2\ \tau_2^{n+1} - \tau^{n+1}$$

$$f_2 \equiv c_1\ \varepsilon_1^{n+1} + c_2\ \varepsilon_2^{n+1} - \varepsilon^{n+1}$$

We know the *overall* mixed cell SIE ε^{n+1} and specific volume τ^{n+1}

Relax toward equilibrium in Δt

$$f_3 \equiv \alpha_1\ \mathcal{P}_1(\varepsilon_1^{n+1},\tau_1^{n+1}) - \alpha_2\ \mathcal{P}_2(\varepsilon_2^{n+1},\tau_2^{n+1}) - (\alpha_3\ p_1^n - \alpha_4\ p_2^n + \alpha_5)$$

$$f_4 \equiv \varepsilon_1^{n+1} - \varepsilon_1^n + P_1\ (\tau_1^{n+1} - \tau_1^n\ ) - [\varepsilon_2^{n+1} - \varepsilon_2^n + P_2\ (\tau_2^{n+1} - \tau_2^n\ )]$$

$\alpha_n = \alpha_n(\tau_k^n, \varepsilon_k^n, u_k^n, \Delta x_{i_{\text{mix}}}, \Delta t, \ldots)$

From Riemann problem

- Recall, in the last equation one must make a modeling choice for the expressions P_1 and P_2.

The Newton iteration is well-conditioned numerically and converges rapidly.

- The Newton iteration can be written:

$$X^{k+1} = X^k - \left[\partial F/\partial X\right]^{-1}_{X^k} \cdot F(X^k)$$

where $F \equiv \left[f_1, f_2, f_3, f_4\right]^{\mathsf{T}}$ and $X \equiv \left[\tau_1^{n+1}, \varepsilon_1^{n+1}, \tau_2^{n+1}, \varepsilon_2^{n+1}\right]^{\mathsf{T}}$

  - The matrix $\partial F/\partial X$ requires pressure derivatives (e.g., $\partial \mathcal{P}_1 / \partial \varepsilon_1$), which can be evaluated for a general EOS.
  - For the pressure-relaxation scheme, the Jacobian does *not* depend on X, i.e., the pressure-relaxation equation does not depend on the t^{n+1} state: $\partial \xi / \partial X = 0$.
  - This matrix has several zero-elements and appears to be well-conditioned for polytropic and stiffened-gas EOSs, for the explicit, implicit, and thermodynamically consistent assumptions.
  - In all cases we have evaluated, this method converges: this is not a proof, *per se*; rather, it is a statement of plausibility.

This model is incorporated into a standard Lagrangian predictor step...

All cells

Artificial viscosity, t^n: $$q_i^n = \begin{cases} 0, & \text{if } u_{i+1}^n - u_i^n \geq 0 \text{ : Expansion} \\ -\nu_1 \rho_i^n c_i^n (u_{i+1}^n - u_i^n) + \nu_2 \rho_i^n (u_{i+1}^n - u_i^n)^2 \end{cases}$$

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

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

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

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

Cell change-in-vol.: $$\Delta V_{i,\text{cell}}^{n+1/2} = V_{i,\text{cell}}^{n+1/2} - V_{i,\text{cell}}^n$$

Cell SIE: $$\varepsilon_i^{n+1/2} = \varepsilon_i^n - (p_i^n + q_i^n) \, \Delta V_{i,\text{cell}}^{n+1/2} \Big/ m_{i,\text{cell}}$$

Cell pressure: The update depends whether the cell is pure or mixed.

Pure cells: $$p_i^{n+1/2} = \mathcal{P}(\varepsilon_i^{n+1/2}, \tau_i^{n+1/2})$$

Mixed cells:

1. Use (i) exact solution (polytropic/stiffened-gas EOS, pressure equilib.) or (iii) Newton (general EOS or pressure relaxation) to solve for $\tau_1^{n+1/2}, \varepsilon_1^{n+1/2}, \tau_2^{n+1/2}, \varepsilon_2^{n+1/2}, p_1^{n+1/2}, p_2^{n+1/2}$
2. Use (i) equilibrated or (ii) "relaxed" value of $p_{i\,\text{mix}}^{n+1/2}$

…followed by a standard Lagrangian corrector step:

All cells

Artificial viscosity, $t^{n+1/2}$: $q_i^{n+1/2} = \begin{cases} 0, & \text{if } u_{i+1}^{n+1/2} - u_i^{n+1/2} \geq 0 : \text{Expansion} \\ -\nu_1 \rho_i^{n+1/2} c_i^{n+1/2} (u_{i+1}^{n+1/2} - u_i^{n+1/2}) \\ \quad + \nu_2 \rho_i^n (u_{i+1}^{n+1/2} - u_i^{n+1/2})^2 \end{cases}$

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

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

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

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

Cell change-in-vol.: $\Delta V_{i,\text{cell}}^{n+1} = V_{i,\text{cell}}^{n+1} - V_{i,\text{cell}}^n$

Cell SIE: $\varepsilon_i^{n+1} = \varepsilon_i^n - \frac{1}{2}(p_i^{n+1/2} + q_i^{n+1/2} + p_i^n + q_i^n)\ \Delta V_{i,\text{cell}}^{n+1} \Big/ m_{i,\text{cell}}$

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

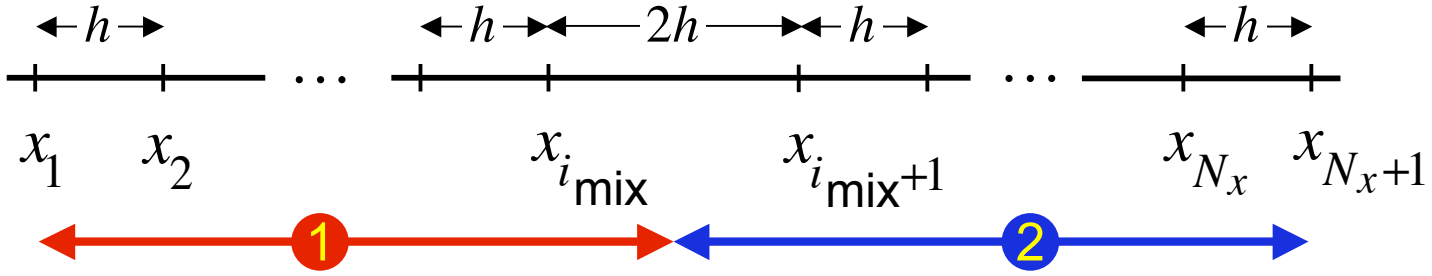
Mixed cells: 1. Use Newton (or exact solution) to solve for

$$\tau_1^{n+1/2},\ \varepsilon_1^{n+1},\ \tau_2^{n+1},\ \varepsilon_2^{n+1},\ p_{i\,\text{mix}}^{n+1}$$

2. Use (i) equilibrated or (ii) "relaxed" $p_{i\,\text{mix}}^{n+1}$

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

- The test problems were run in a similar fashion:
  - N_x zones on $x_{\min} \le x < x_{\max}$ with $\Delta x_i = h$, $i \neq i_{\text{mix}}$
  - One mixed cell for $i = i_{\text{mix}}$ with $\Delta x_{i_{\text{mix}}} = 2h$



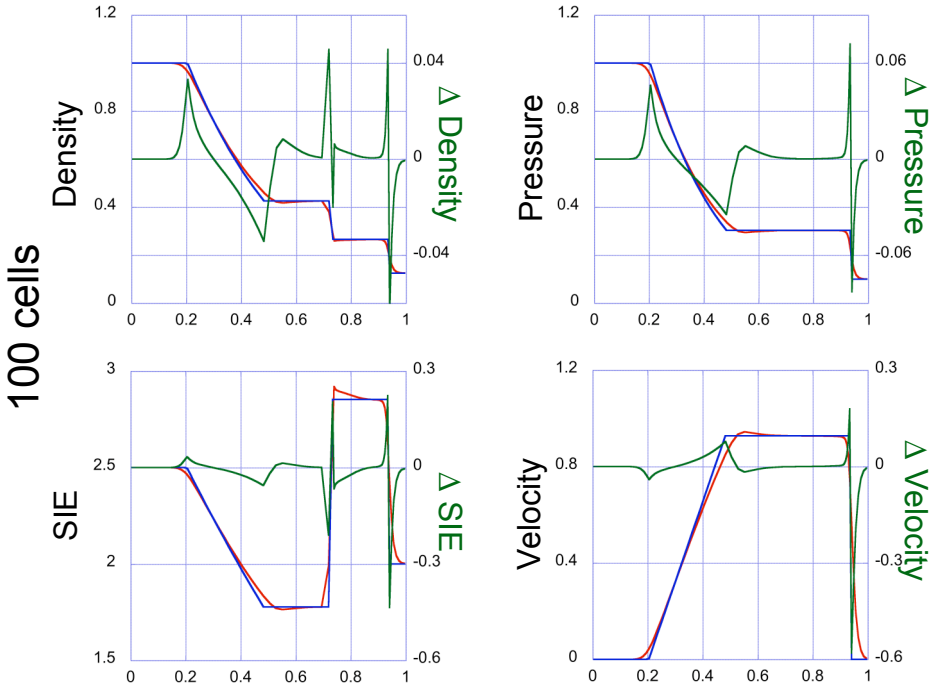
  - The fictitious mixed-cell interface is assigned at the center of mixed cell, with no explicit mass-matching
    - This information is used, e.g., to calculate the mixed-cell mass fractions.
- Graphical results for the test problems include:
  - "Snapshots": fixed-in-time, spatial solution over the whole mesh
  - "Histories": fixed-in-space, temporal solution only in the mixed cell

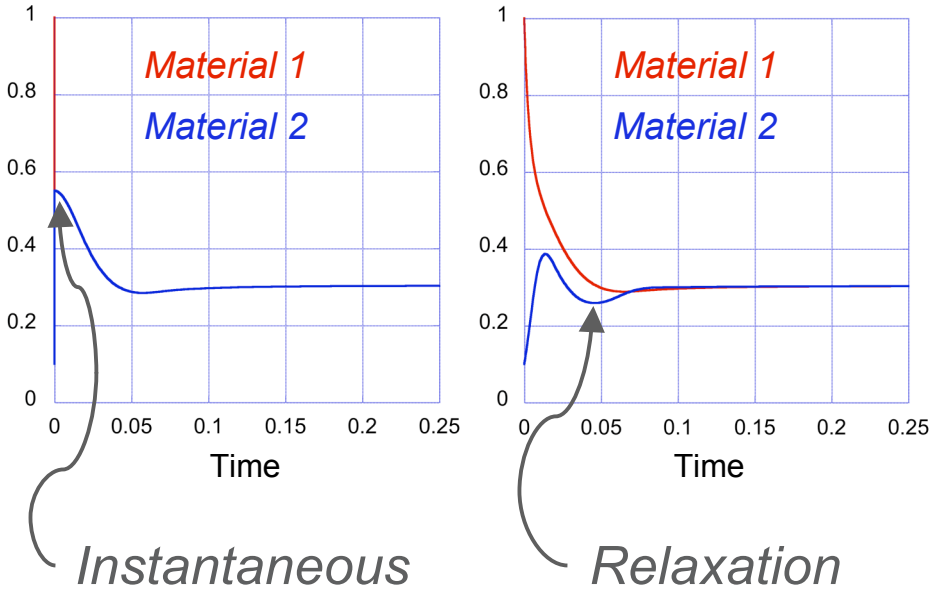
The results for the Sod shock tube suggest that this approach is reasonable.

- Sod problem initial conditions:

$$(\rho,p,u,\gamma) = \begin{cases} (1.0,\ 1.0,\ 0.0, 1.4), & 0 \le x < 0.5 \\ (0.125, 0.1, 0.0, 1.4), & 0.5 < x \le 1.0 \end{cases} \qquad t_{\text{final}} = 0.25$$

- *FE*: "Exact" mixed-cell sol'n
  |FE - Newton| < 1.e-10
- *TC*: Instan's. vs. Relax'n:
  Mixed Cell Pressures





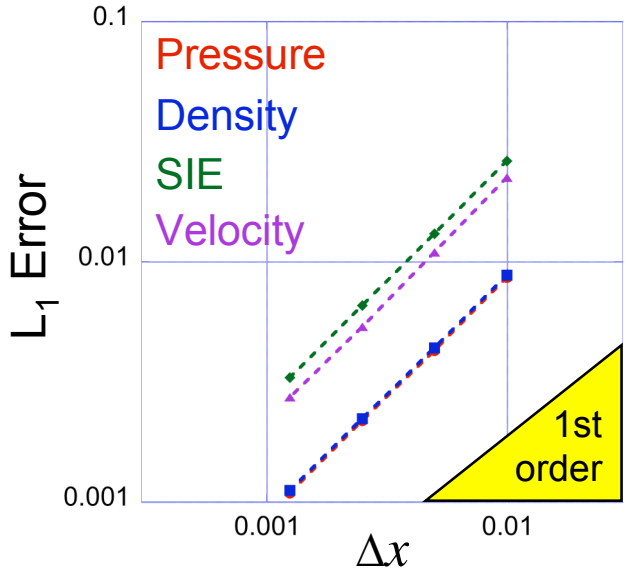
"Closed-form" – *Computed* = *Difference*

– Similar results for all closure models.

The method shows overall first-order convergence results for the Sod problem.

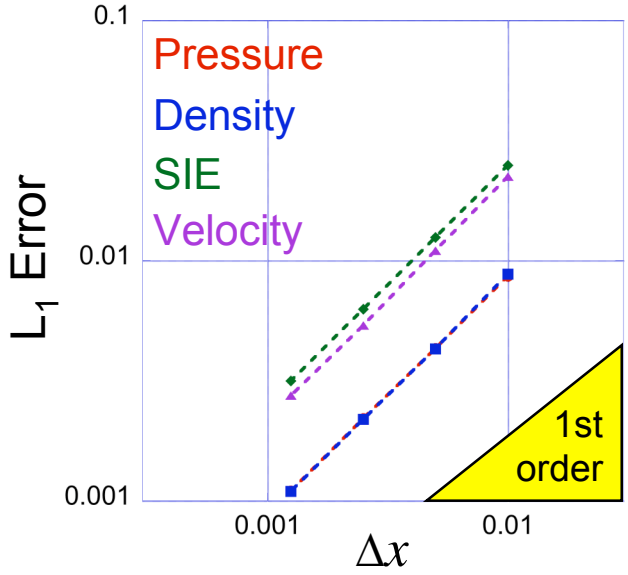
- Make the Ansatz: $\left\| y^{\text{exact}} - y^{\text{computed}} \right\|_1 = A(\Delta x)^{\sigma} + \cdots$

Exact FE



Variable	A	σ
Pressure	0.82	0.99
Density	0.84	0.99
SIE	2.58	1.00
Velocity	2.35	1.01

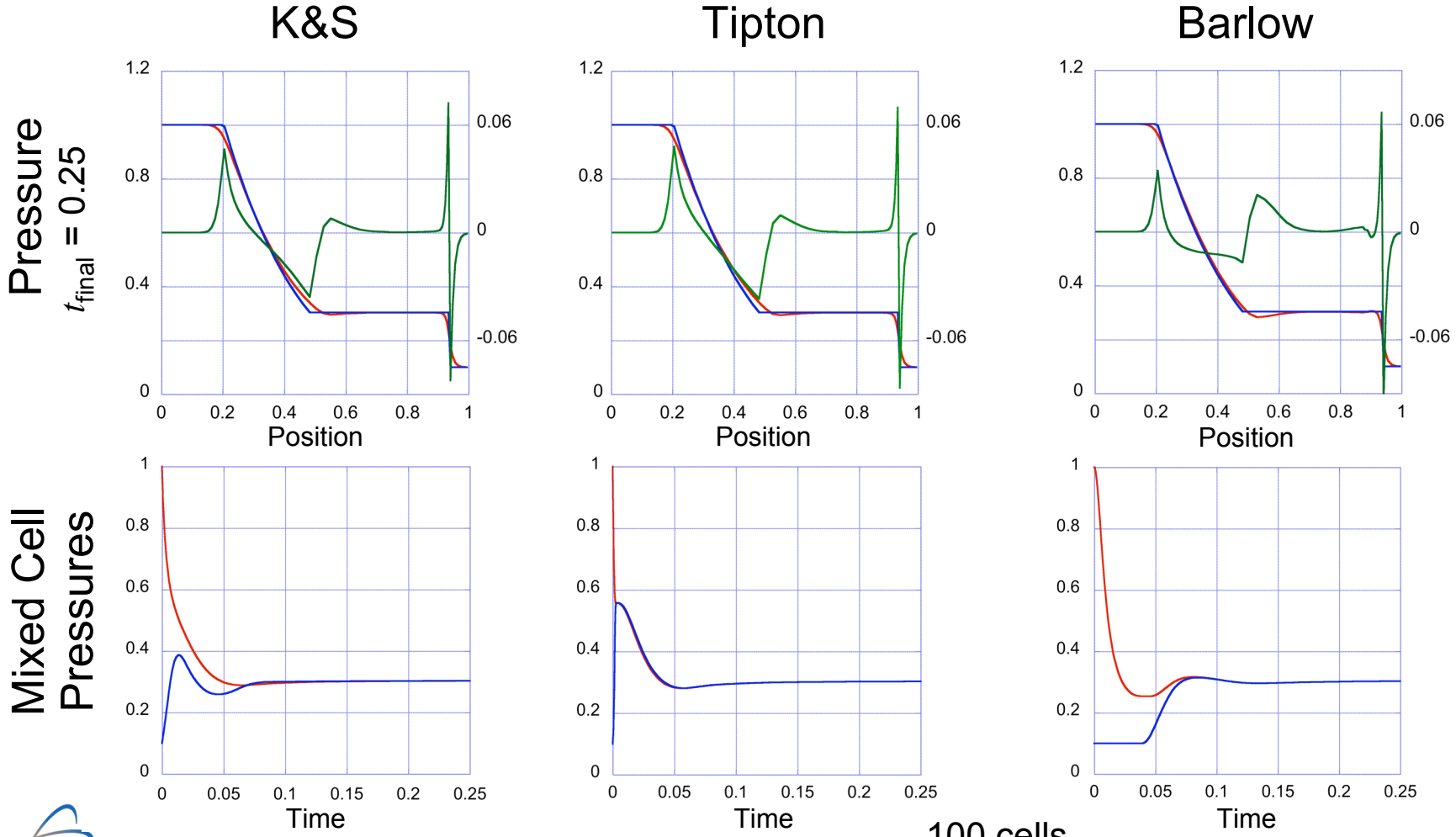
Newton-Relax'n FE



Variable	A	σ
Pressure	0.82	0.99
Density	0.87	1.00
SIE	2.43	1.00
Velocity	2.33	1.01

Our results compare favorably with Tipton's and Barlow's methods for the Sod shock tube.

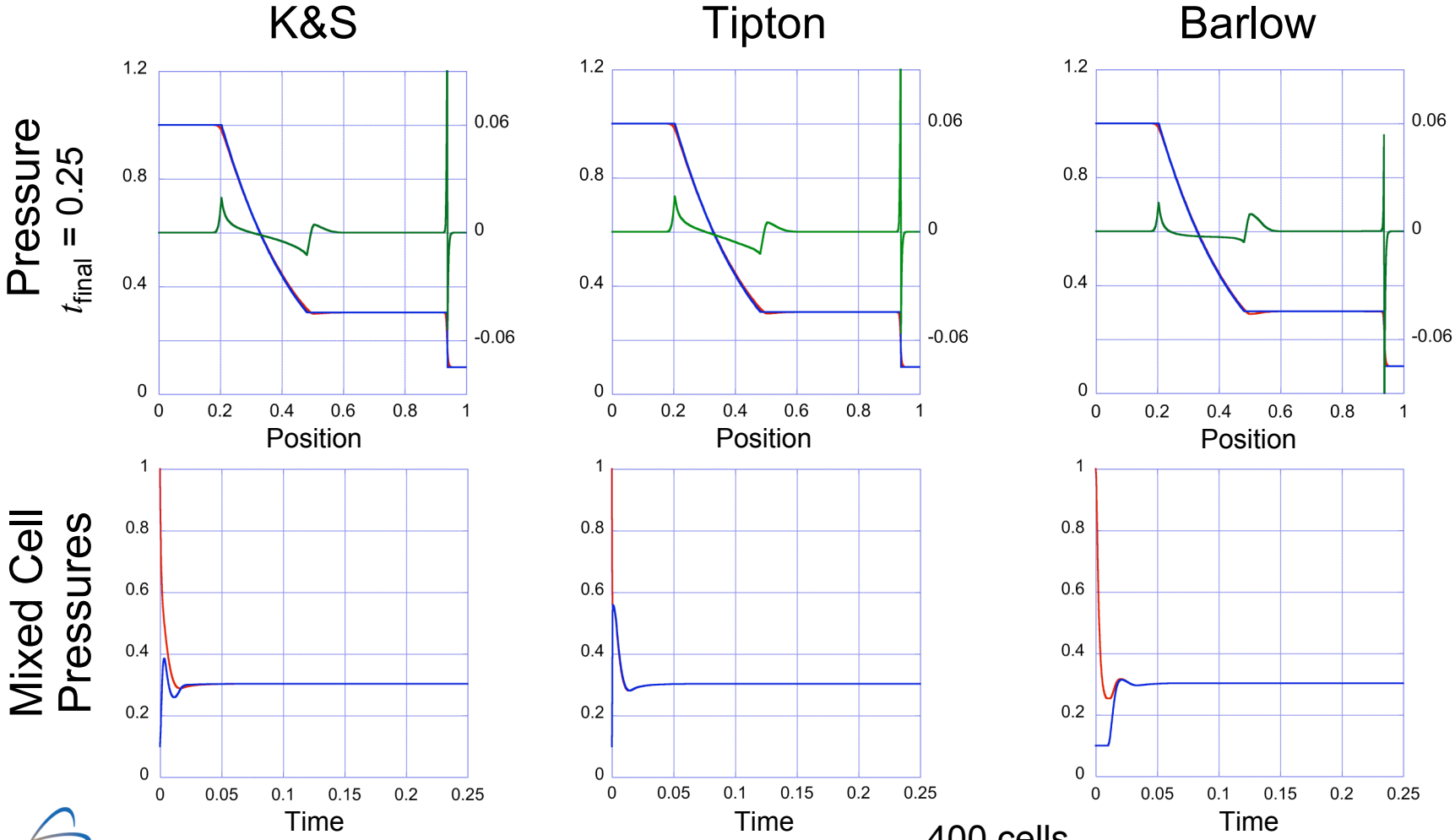
- Both Barlow and Tipton use pressure relaxation schemes.



LA-UR-07-5900

Increasing mesh resolution by a factor of four implies a shorter relaxation time.

- It also implies sharper features:



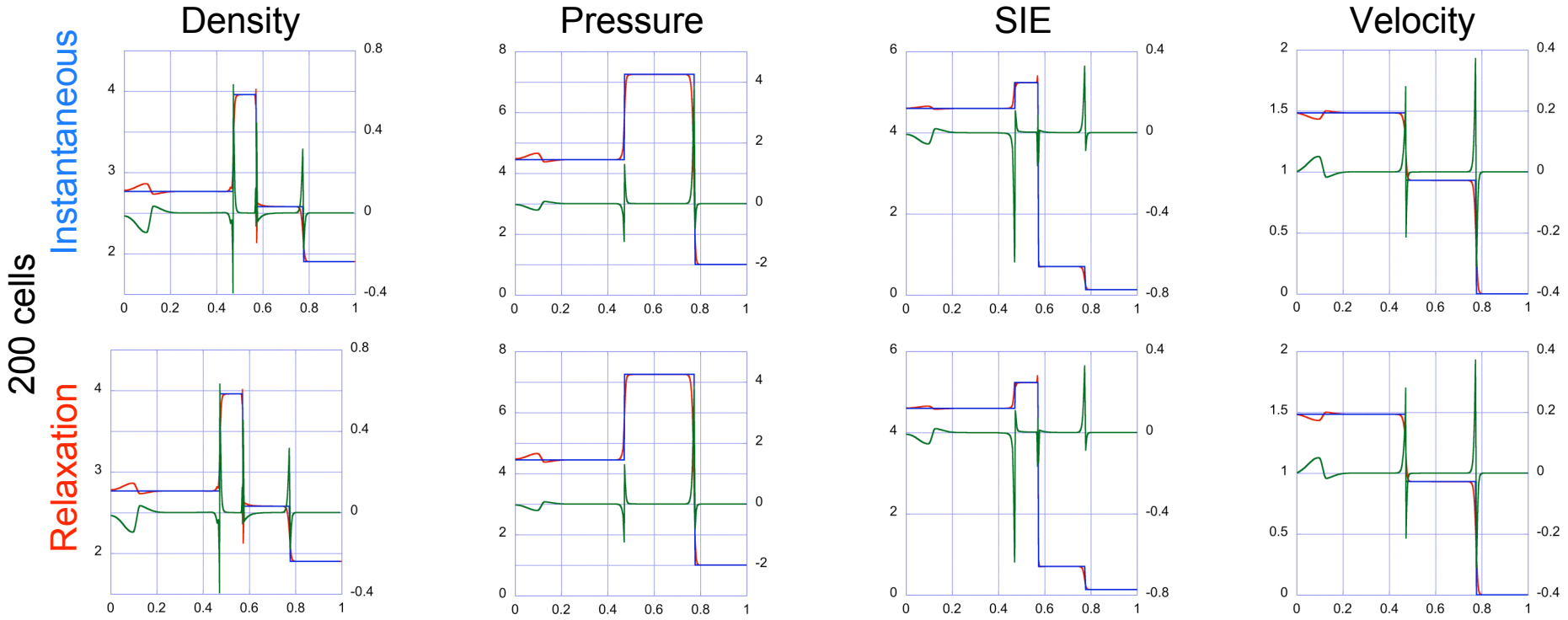
This shock-contact problem* tests the behavior through a pure, two-material contact.

- Two-material, γ-law gas problem, rightward shockwave

$$(\rho,p,u,\gamma) = \begin{cases} (2.76,\ 4.45,\ 1.48, 1.35), & 0<x<0.1 \\ (1.0,\ \ 1.0,\ \ 0.0, 1.35), & 0.1<x<0.5 \\ (1.9,\ \ 1.0,\ \ 0.0, 5.0), & 0.5<x<1 \end{cases}$$

Mach 2 shock

$t_{\text{final}} = 0.25$



"Closed-form" – Computed = Difference

* J.W. Banks et al. "A high-resolution Godunov method for compressible multi-material flow on overlapping grids," *J. Comp. Phys.* **150**, 425–467 (2007).

This shock-contact problem allows us to test all of the exact equilibration closure solutions.

- Two closure solutions produce invalid solutions for this multi-material, multi-γ test problem:

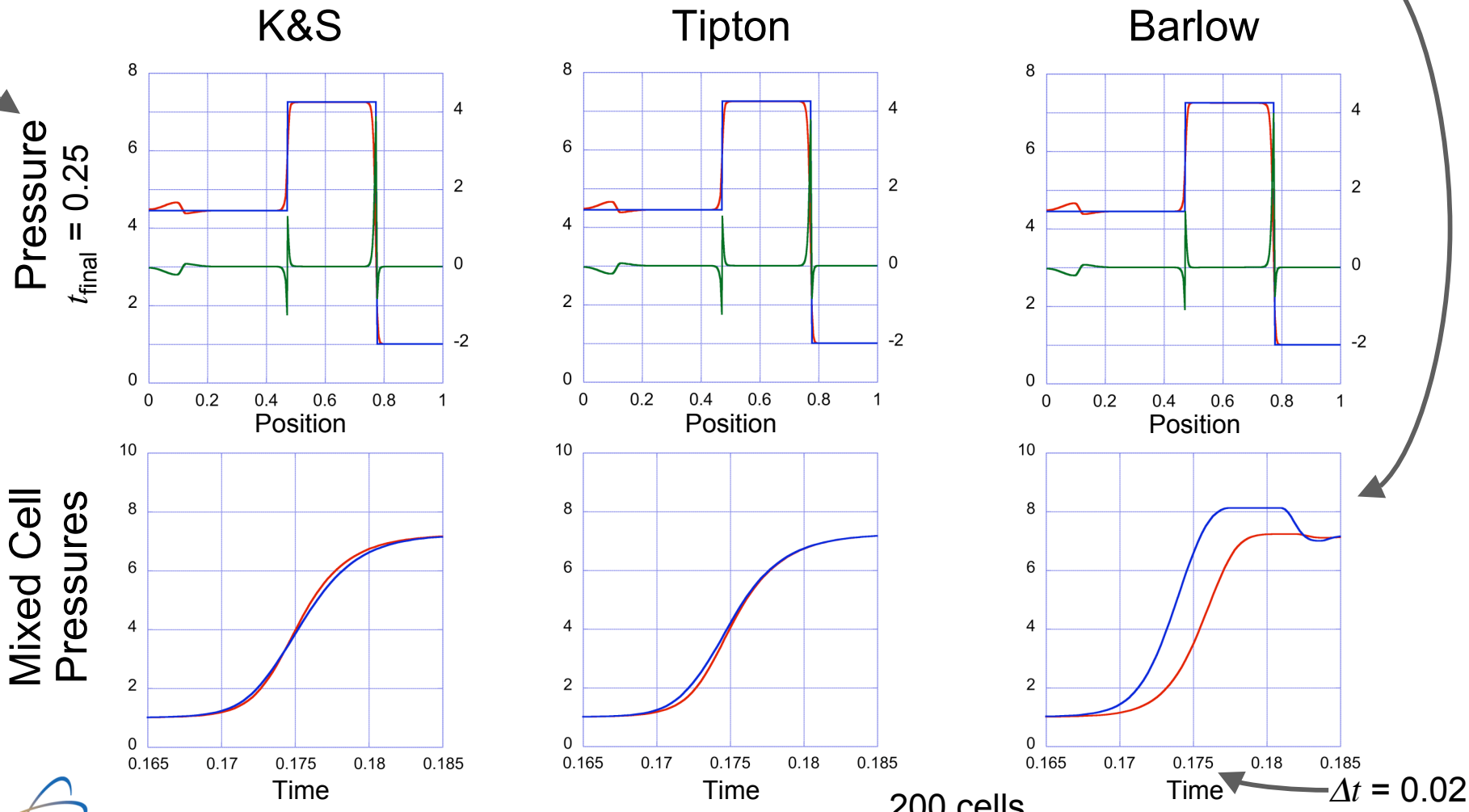
Fully Explicit #1	Fully Explicit #2	Fully Implicit	Therm. Cons. #1	Therm. Cons. #2
				
Density, sound speed negative on cycle 1	Runs to completion	Runs to completion	Density, sound speed negative on cycle 1	Runs to completion

- The mathematics here might be telling us something — is there a removable singularity (that wasn't removed)?
  - This is a subject for further investigation…

LA-UR-07-5900

The shock-contact problem shows little difference among the methods.

- The snapshots are similar.
- The time-histories differ.

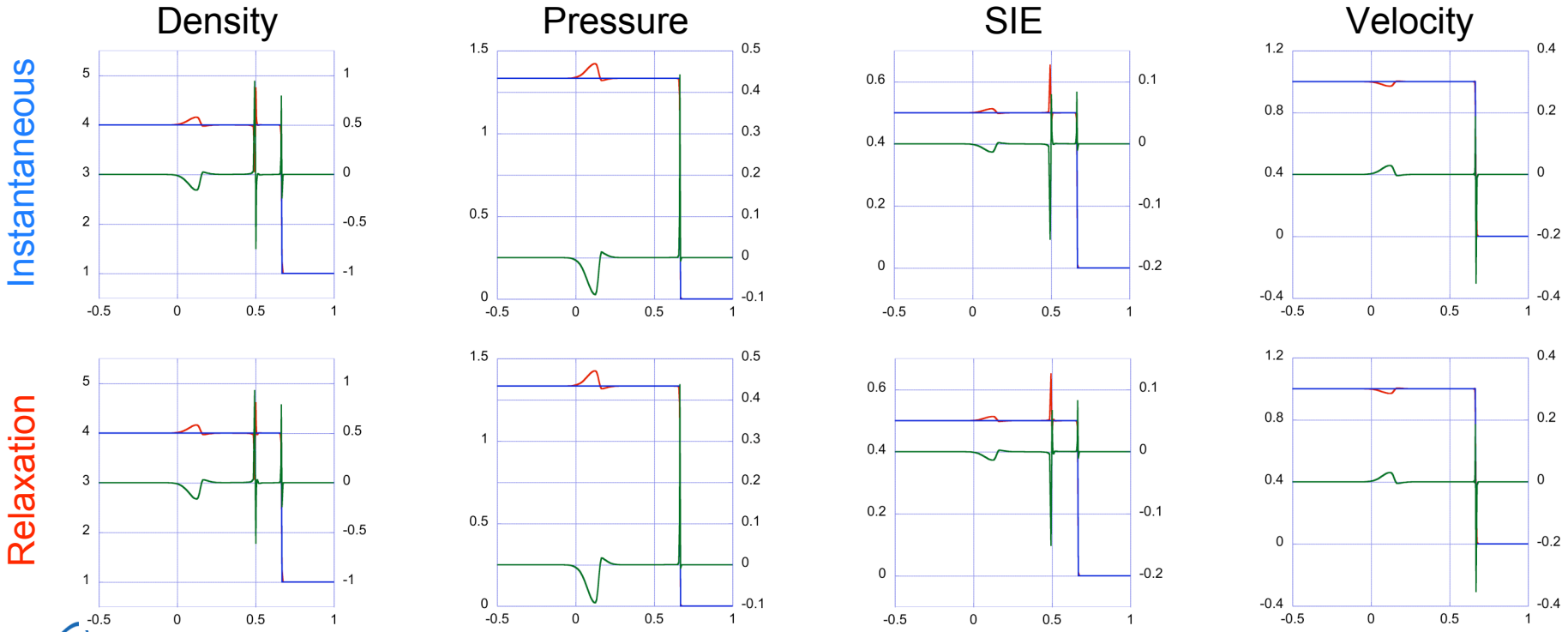


The moving-shock problem tests the basic strong-shock propagation capabilities.

- One-material, 2×10^4-strength shock propagation:

$$(\rho,p,u,\gamma) = \begin{cases} (4.0,\ 4/3,\ \ \ 1.0,\ 5/3), & -1\le x<0 \\ (1.0,\ 2/3\times10^{-4},\ 0.0,\ 5/3), & 0<x\le 1 \end{cases} \qquad u_{\text{Left}} = 1.0,\quad t_{\text{final}} = 0.5$$

- *TC*: "Comparison of instantaneous and relaxation results:



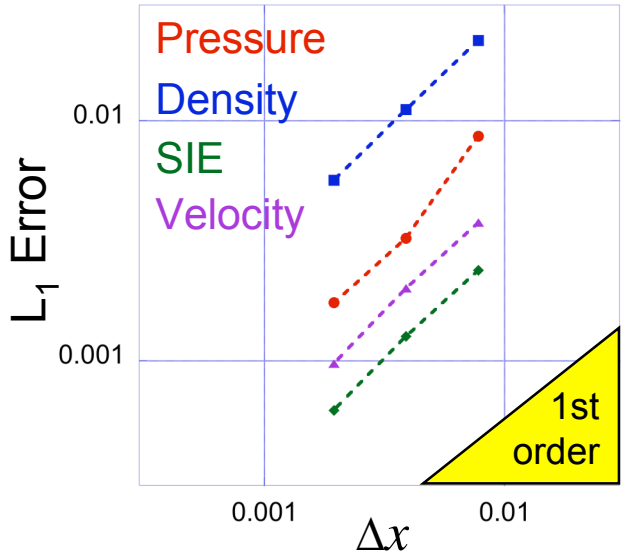
"Closed-form" – Computed = Difference

256 cells

The moving-shock problem also exhibits overall first-order convergence.

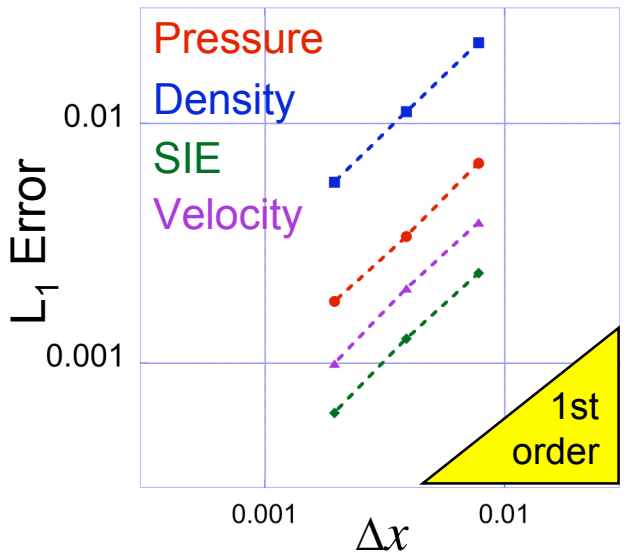
- Make the Ansatz: $\left\| y^{\text{exact}} - y^{\text{computed}} \right\|_1 = A(\Delta x)^{\sigma} + \cdots$

Exact TC



Variable	A	σ
Pressure	2.17	1.15
Density	2.34	0.97
SIE	0.27	0.97
Velocity	0.43	0.98

Newton-Relax'n TC

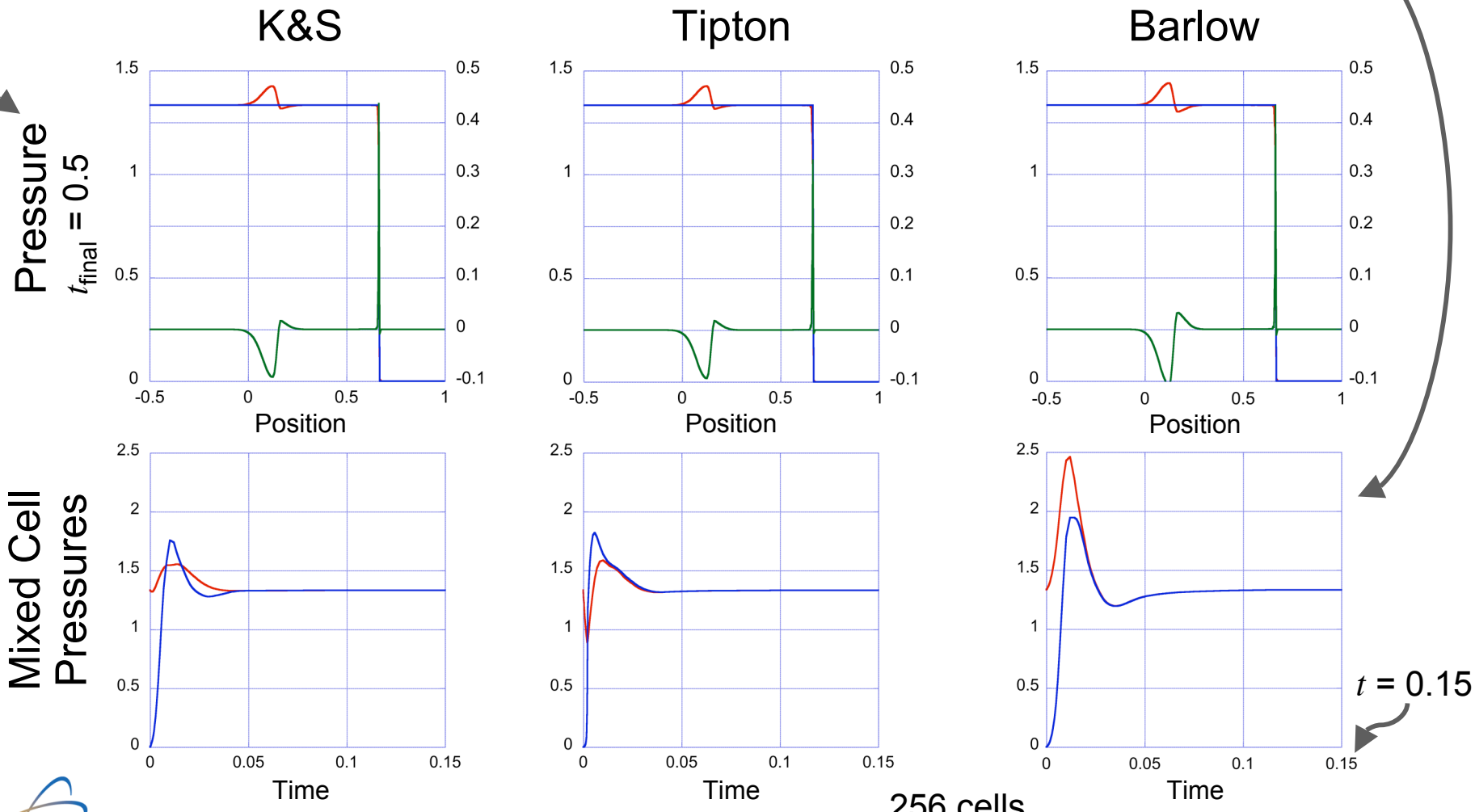


Variable	A	σ
Pressure	0.70	0.96
Density	2.36	0.97
SIE	0.27	0.97
Velocity	0.45	0.98

LA-UR-07-5900

The moving-shock problem exhibits some minor differences among the methods.

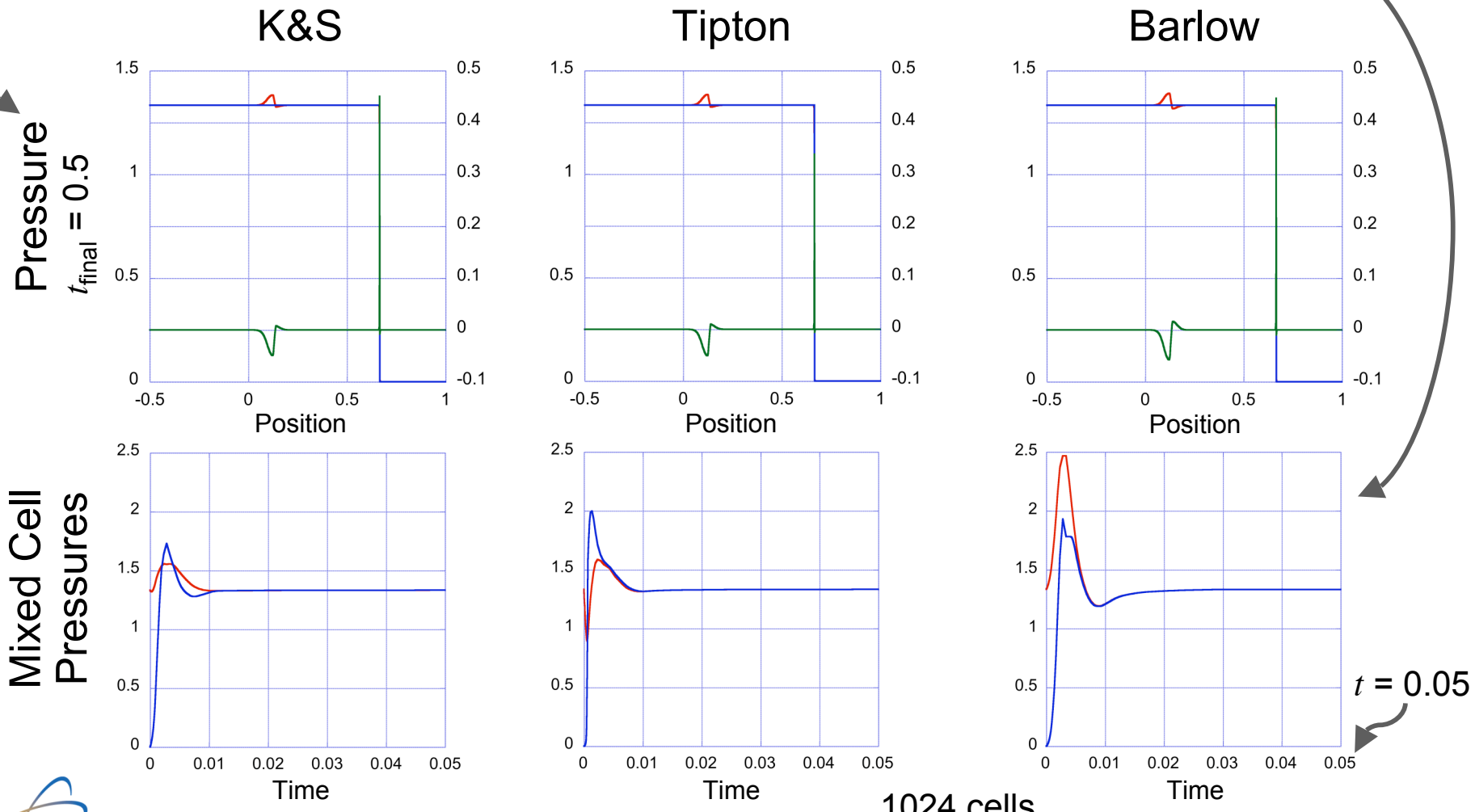
- The snapshots are similar.
- The time-histories differ.



LA-UR-07-5900

Finer (4x) resolution on the moving-shock problem reveals only minor differences.

- Minor differences.
- *Early*-time differences.

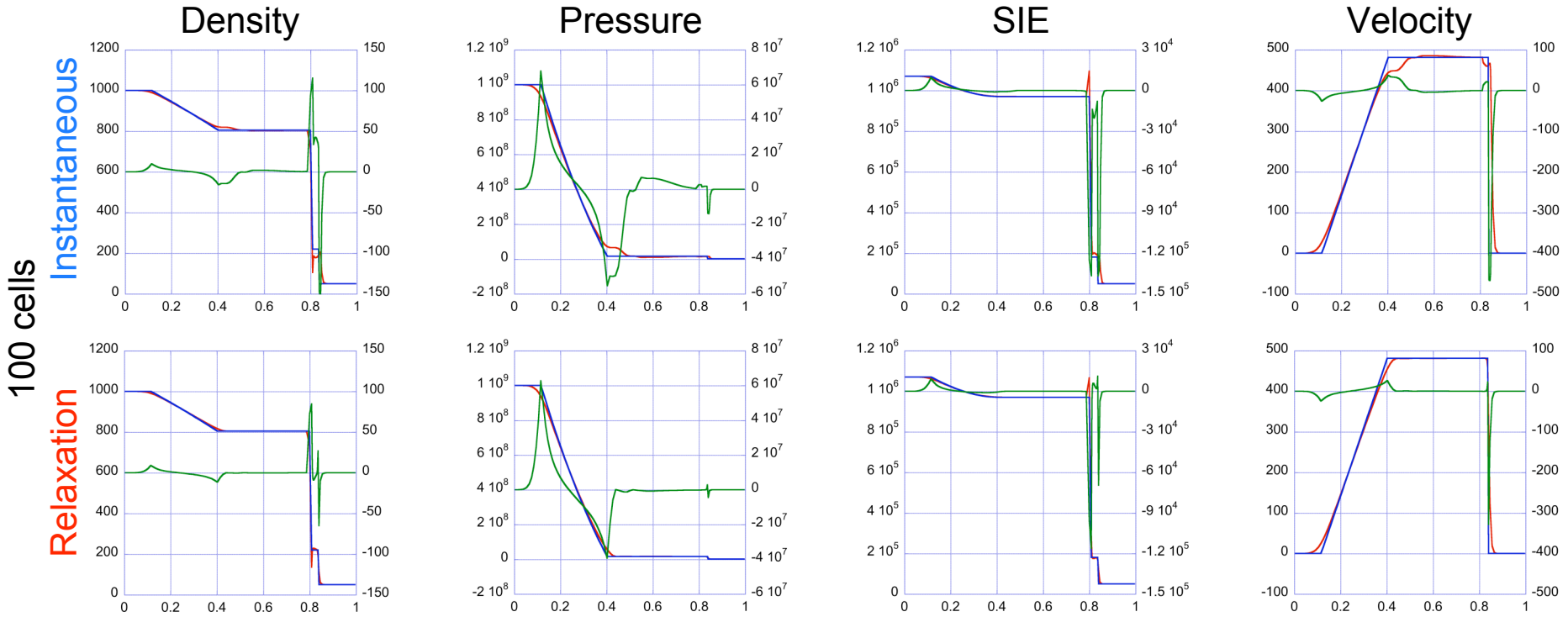


A water-air shock tube has become a *de facto* standard for multimaterial hydro solvers.

- Water-air shock tube problem* with stiffened gas EOS:

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

- *TC*: Differences in post-shock and near-rarefaction results.

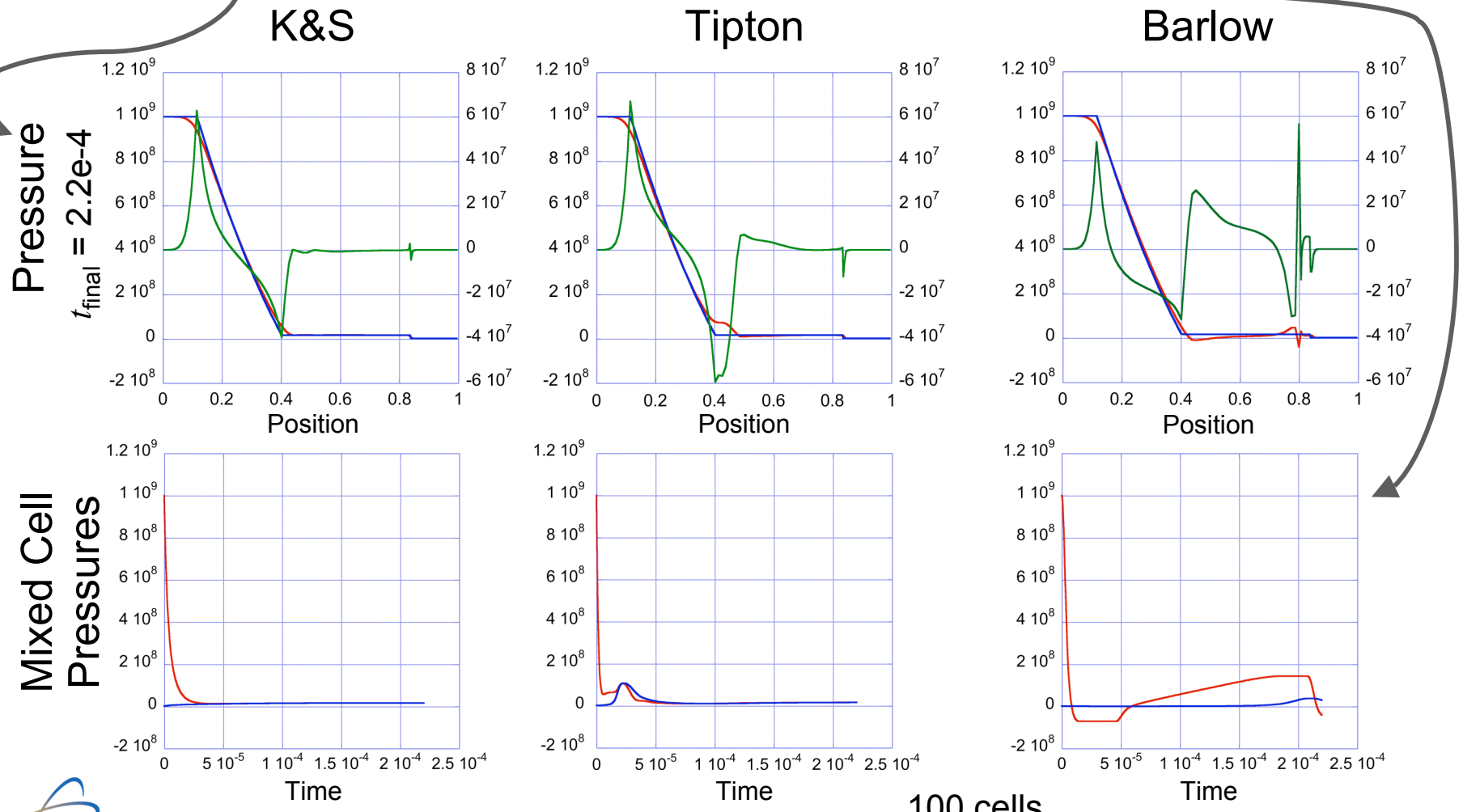


"Closed-form" – Computed = Difference

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

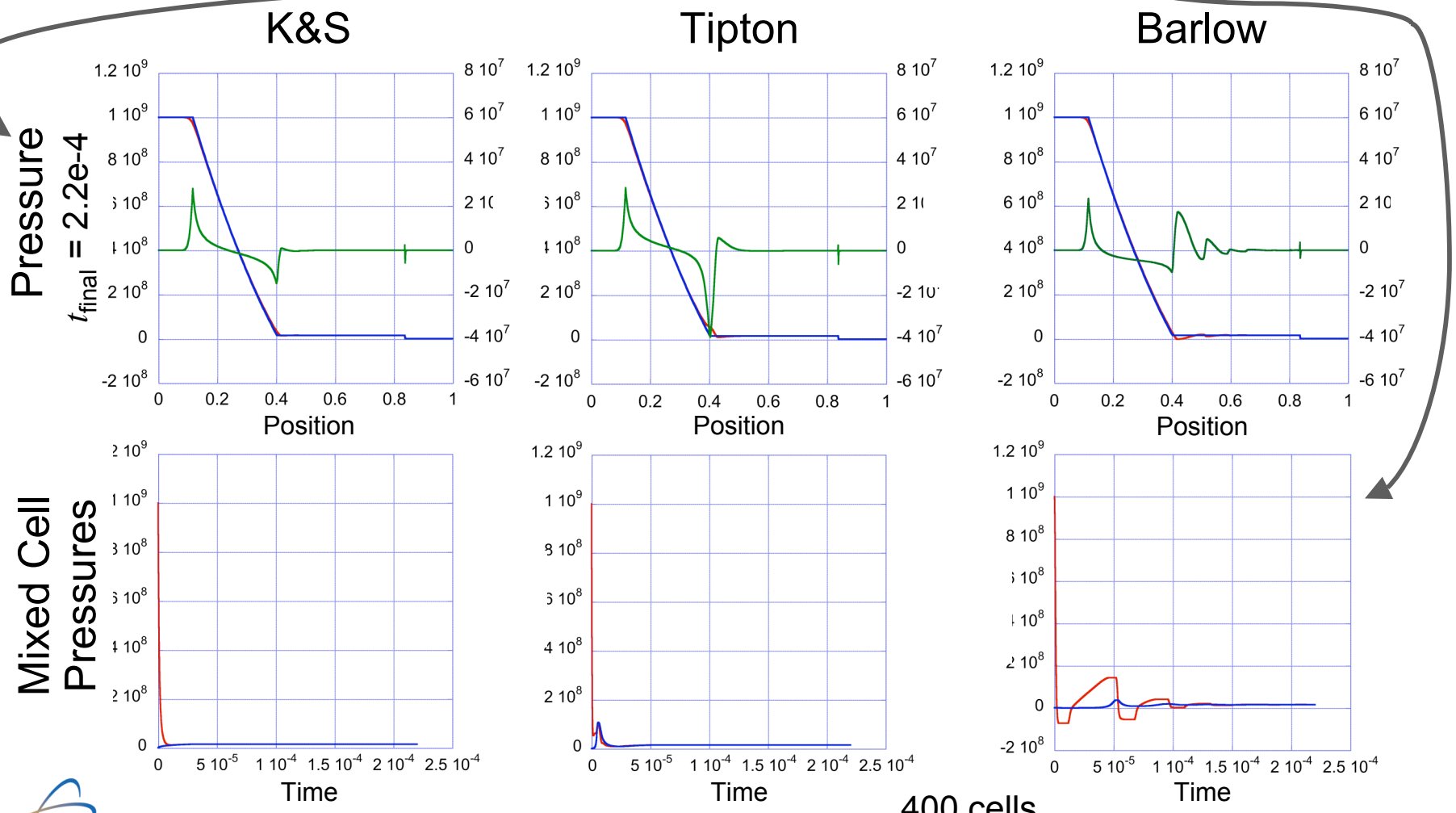
The water-air shock tube problem highlights some differences among the methods.

- The snapshots and time-histories differ among all methods.



Again, increasing mesh resolution by a factor of four implies a shorter relaxation time.

- The water-air shock snapshots and time-histories still differ.



There are advantages, disadvantages, and open questions about this approach.

- **Exact solutions** of three mixed-cell equilibrium closure models permit confirmation of Newton's method coding (but there are open questions).
- **Riemann-problem-based pressure-relaxation model** for mixed cells:
  - This breaks the assumption of instantaneous pressure equilibrium.
  - It uses a physics-motivated approach to evolve the mixed cell states.
  - It is sufficiently general for a tabular EOS.
  - Use the form of the K-S pressure relaxation equations (1) to better understand and/or (2) to improve other models (Tipton, Barlow).
- **Limitations** of this model:
  - Slower: (1) Riemann-solve (→approx.), (2) Newton's method (→1-step).
  - Extension to 2-D or 3-D would require further approximations.
    - E.g., how does one address the issue of interface orientation?
  - How does one deal with many (>2) materials?
- **Rigorous comparison** of different methods on well-defined test problems allows careful examination of important flow situations.