On the Construction of High-Order and Exact Pressure Equilibrium Schemes for Arbitrary Equations of State

Christopher DeGrendele[1,3], Nguyen Ly[2], Francois Cadieux[1], Michael Barad[1], Dongwook Lee[3], Jared Duensing[1]

[1] NASA Ames Research Center

[2]Analytical Mechanics Associates

[3]University of California, Santa Cruz

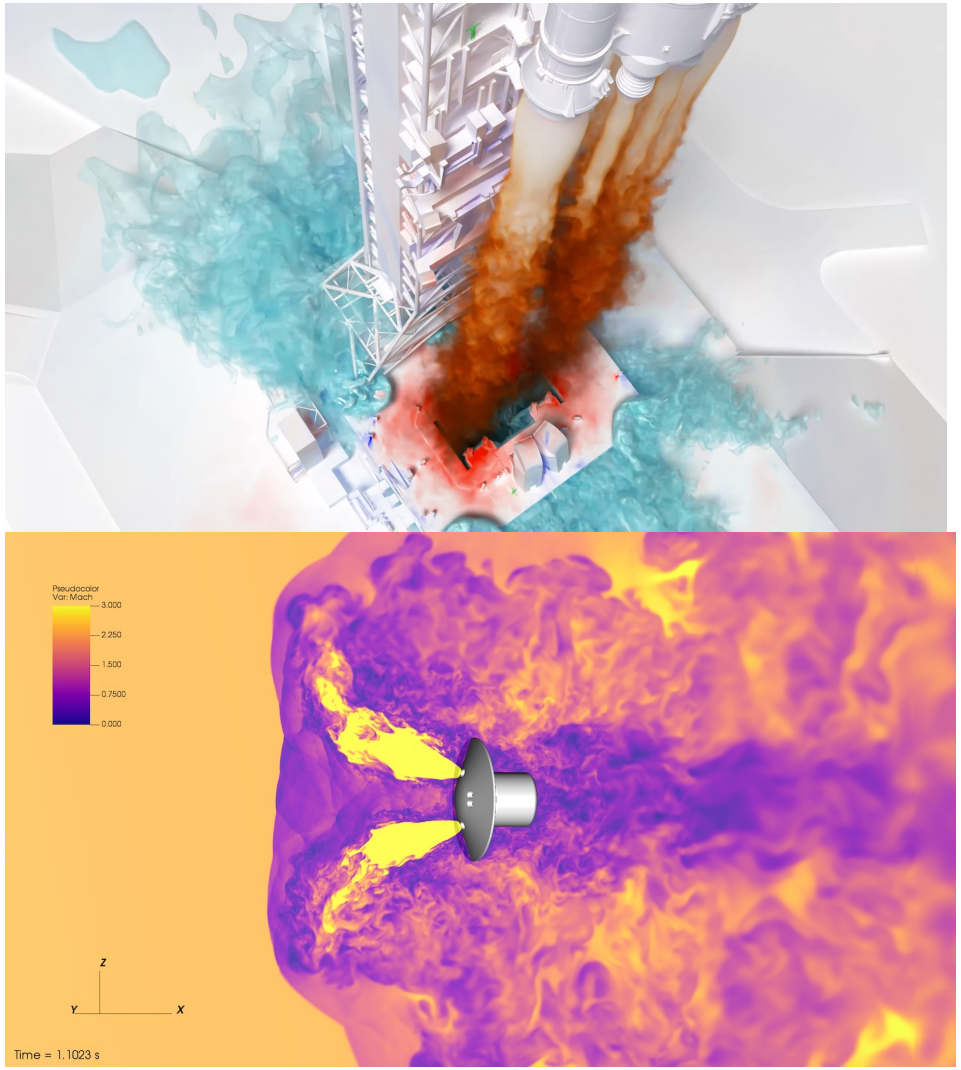
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Motivation

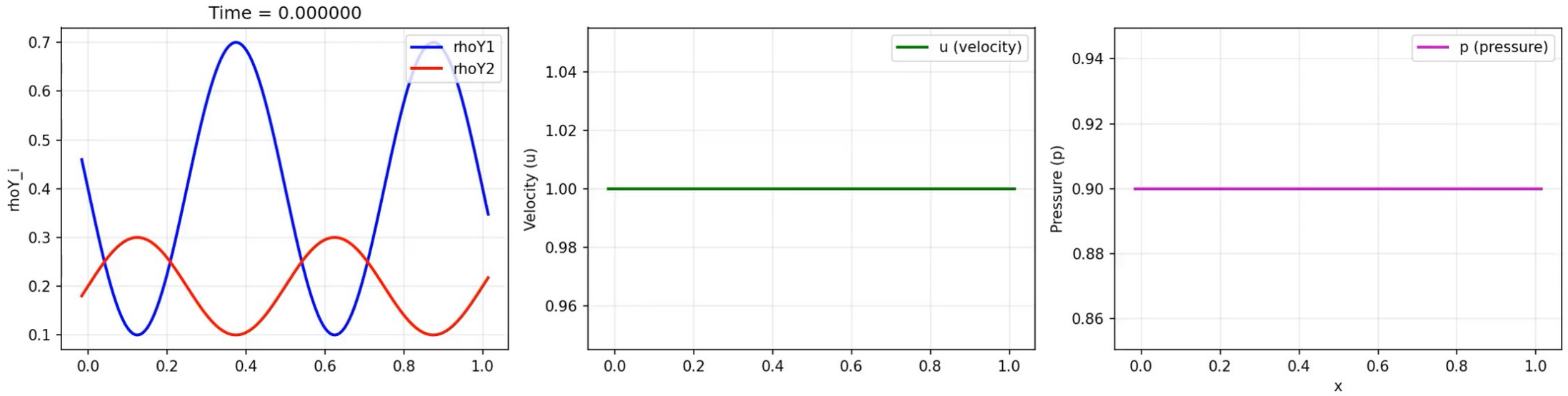
- Multi-species and multi-phase flows are used to model many physical phenomena across a variety of fields.

- In the Launch Ascent Vehicle Aerodynamics (LAVA) group, we use multi-fluid simulations for:
  - Launchpad environment simulations
  - Vehicle ascent/descent and plume vehicle interactions
  - Nozzle driven and exhaust flow configurations

- Long time stability and accuracy of these multi-fluid simulations are compromised by spurious pressure oscillations



Motivation



Two-species advection flow, KEEP scheme

Existing Methods

Non-Conservative

Non-conservative pressure-based methods *Multicomponent Flow Calculations by a Consistent Primitive Algorithm (Karni, 1994)*	Evolve pressure directly to enforce equilibrium

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This work	Arbitrary EOS, exact Multiphase extension

Outline

Single-species and Multi-species

1. **Pressure In-Equilibrium Analysis**
2. Spatially Exact PEP Scheme
3. Results

Multi-phase

4. Augmented 5-Equation Formulation
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Two-Species 1D Euler Equations

$$
\begin{aligned}
\frac{\partial(\rho Y_1)}{\partial t} + \frac{\partial(\rho Y_1 u)}{\partial x} &= 0 \\
\frac{\partial(\rho Y_2)}{\partial t} + \frac{\partial(\rho Y_2 u)}{\partial x} &= 0 \\
\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u u + p)}{\partial x} &= 0 \\
\frac{\partial(\rho E)}{\partial t} + \frac{\partial\left[(\rho E + p)u\right]}{\partial x} &= 0,
\end{aligned}
$$

Fluxes

$$
\begin{aligned}
F_{\rho Y_1}|_m &= \frac{C_1|_{m+\frac{1}{2}} - C_1|_{m-\frac{1}{2}}}{\Delta x} \\
F_{\rho Y_2}|_m &= \frac{C_2|_{m+\frac{1}{2}} - C_2|_{m-\frac{1}{2}}}{\Delta x} \\
F_{\rho u}|_m &= \frac{M|_{m+\frac{1}{2}} - M|_{m-\frac{1}{2}}}{\Delta x} + \frac{\Pi|_{m+\frac{1}{2}} - \Pi|_{m-\frac{1}{2}}}{\Delta x} \\
F_{\rho E}|_m &= \frac{K|_{m+\frac{1}{2}} - K|_{m-\frac{1}{2}}}{\Delta x} + \frac{I|_{m+\frac{1}{2}} - I|_{m-\frac{1}{2}}}{\Delta x} + \frac{S|_{m+\frac{1}{2}} - S|_{m-\frac{1}{2}}}{\Delta x}
\end{aligned}
$$

Pressure-Equilibrium Property

- The problem is to maintain pressure-equilibrium through the numerical time stepping:

  Define the choice of mid-point values $\rho Y_1|_{m+\frac{1}{2}}, \rho Y_2|_{m+\frac{1}{2}}, \rho|_{m+\frac{1}{2}}, \rho e|_{m+\frac{1}{2}}$

  such that after one numerical time step

$$\text{If} \quad \begin{cases} u|_m^n = U_0 \\ p|_m^n = p_0 \end{cases} \quad \text{then} \quad \begin{cases} u|_m^{n+1} = U_0 \\ p|_m^{n+1} = p_0 \end{cases}$$

- Approach: Expand the balanced primitives w.r.t. conservative variables

- For example: Velocity equilibrium condition

$$u|_m^{n+1} - u|_m^n = \left(\frac{\partial u}{\partial \rho u}\right)_\rho \Bigg|_m^n (\rho u|_m^{n+1} - \rho u|_m^n) + \left(\frac{\partial u}{\partial \rho}\right)_{\rho u} \Bigg|_m^n (\rho|_m^{n+1} - \rho|_m^n) + \text{H.O.}$$

  - This condition is automatically satisfied (to first order in time) if

$$\rho|_{m+\frac{1}{2}} \equiv \rho Y_1|_{m+\frac{1}{2}} + \rho Y_2|_{m+\frac{1}{2}},$$

Pressure-Equilibrium Condition

- We can analyze pressure in the same way: $p = f(\rho e, \rho Y_1, \rho Y_2)$

$$p_m^{n+1} - p_m^n = \left(\frac{\partial p}{\partial \rho e}\right)_m^n \left(\rho e_m^{n+1} - \rho e_m^n\right) + \sum_{i=1}^{2} \left(\frac{\partial p}{\partial \rho Y_i}\right)_m^n \left((\rho Y_i)_m^{n+1} - (\rho Y_i)_m^n\right) + O(\Delta t^2)$$

$$\rho e_m^{n+1} - \rho e_m^n = -F_{\rho E,m}^n \Delta t + u_m^n F_{\rho u,m}^n \Delta t - \frac{1}{2}(u_m^n)^2 F_{\rho,m}^n \Delta t + O(\Delta t^2)$$

$$(\rho Y_i)_m^{n+1} - (\rho Y_i)_m^n = -U_0 \frac{\Delta t}{\Delta x}\left((\rho Y_i)_{m+\frac{1}{2}}^n - (\rho Y_i)_{m-\frac{1}{2}}^n\right) + O(\Delta t^2)$$

Pressure-Equilibrium (PEQ) Property

- After some algebra

$$\rho e|_{m+\frac{1}{2}} - \rho e|_{m-\frac{1}{2}} = \sum_{i=1}^{N} \left(\frac{\partial \rho e}{\partial \rho Y_i} \right)_{\rho Y_{j\neq i}, p} \Bigg|_{m} \left[(\rho Y_i)_{m+\frac{1}{2}} - (\rho Y_i)_{m-\frac{1}{2}} \right]$$

- We can split this into the left and right cell interface

$$\rho e|_{m+\frac{1}{2}} - \rho e|_{m} = \sum_{i=1}^{N} \left(\frac{\partial \rho e}{\partial \rho Y_i} \right)_{\rho Y_{j\neq i}, p} \Bigg|_{m} \left(\rho Y_i|_{m+\frac{1}{2}} - \rho Y_i|_{m} \right)$$

$$\rho e|_{m+1} - \rho e|_{m+\frac{1}{2}} = \sum_{i=1}^{N} \left(\frac{\partial \rho e}{\partial \rho Y_i} \right)_{\rho Y_{j\neq i}, p} \Bigg|_{m+1} \left(\rho Y_i|_{m+1} - \rho Y_i|_{m+\frac{1}{2}} \right).$$

Interface-Local PEQ Criterion

To satisfy the PEQ criterion we must satisfy

$$\rho e|_{m+\frac{1}{2}} - \rho e|_m = \sum_{i=1}^{N} \left(\frac{\partial \rho e}{\partial \rho Y_i} \right)_{\rho Y_{j\neq i}, p} \Bigg|_m \left(\rho Y_i|_{m+\frac{1}{2}} - \rho Y_i|_m \right)$$

$$\rho e|_{m+1} - \rho e|_{m+\frac{1}{2}} = \sum_{i=1}^{N} \left(\frac{\partial \rho e}{\partial \rho Y_i} \right)_{\rho Y_{j\neq i}, p} \Bigg|_{m+1} \left(\rho Y_i|_{m+1} - \rho Y_i|_{m+\frac{1}{2}} \right).$$

2 equations, 3 unknowns

APEC Method

APEC takes the two constraints

$$\rho e|_{m+\frac{1}{2}} - \rho e|_m = \sum_{i=1}^{N} \left(\frac{\partial \rho e}{\partial \rho Y_i} \right)_{\rho Y_{j\neq i}, p} \Bigg|_m \left(\rho Y_i|_{m+\frac{1}{2}} - \rho Y_i|_m \right)$$

$$\rho e|_{m+1} - \rho e|_{m+\frac{1}{2}} = \sum_{i=1}^{N} \left(\frac{\partial \rho e}{\partial \rho Y_i} \right)_{\rho Y_{j\neq i}, p} \Bigg|_{m+1} \left(\rho Y_i|_{m+1} - \rho Y_i|_{m+\frac{1}{2}} \right).$$

And combines them via subtraction to get

$$\rho e|^{\text{APEC}}_{m+\frac{1}{2}} = \frac{\rho e|_m + \rho e|_{m+1}}{2} + \frac{1}{2} \sum_{i=1}^{N} \left[\left(\frac{\partial \rho e}{\partial \rho Y_i} \right)_{\rho Y_{j\neq i}, p} \Bigg|_m \left(\rho Y_i|_{m+\frac{1}{2}} - \rho Y_i|_m \right) - \left(\frac{\partial \rho e}{\partial \rho Y_i} \right)_{\rho Y_{j\neq i}, p} \Bigg|_{m+1} \left(\rho Y_i|_{m+1} - \rho Y_i|_{m+\frac{1}{2}} \right) \right].$$

APEC Method

This is now a single constraint, with 3 unknowns.

$$\rho e|^{\text{APEC}}_{m+\frac{1}{2}} = \frac{\rho e|_m + \rho e|_{m+1}}{2} + \frac{1}{2}\sum_{i=1}^{N}\left[\left(\frac{\partial \rho e}{\partial \rho Y_i}\right)_{\rho Y_{j\neq i},p}\Bigg|_m \left(\rho Y_i|_{m+\frac{1}{2}} - \rho Y_i|_m\right) - \left(\frac{\partial \rho e}{\partial \rho Y_i}\right)_{\rho Y_{j\neq i},p}\Bigg|_{m+1} \left(\rho Y_i|_{m+1} - \rho Y_i|_{m+\frac{1}{2}}\right)\right].$$

APEC chooses to solve for ρe and we are left with an arbitrary choice for face value of mass fractions

$$\rho Y_i|^{\text{APEC}}_{m+\frac{1}{2}} = \frac{\rho Y_i|_m + \rho Y_i|_{m+1}}{2}.$$

APEC Method

Observation: APEC acts as a “correction” to the ρe interface between cells m and m+1

$$\rho e|^{\text{APEC}}_{m+\frac{1}{2}} = \frac{\rho e|_m + \rho e|_{m+1}}{2} + \frac{1}{2}\sum_{i=1}^{N}\left[\left(\frac{\partial \rho e}{\partial \rho Y_i}\right)_{\rho Y_{j\neq i},p}\Bigg|_m \left(\rho Y_i|_{m+\frac{1}{2}} - \rho Y_i|_m\right) - \left(\frac{\partial \rho e}{\partial \rho Y_i}\right)_{\rho Y_{j\neq i},p}\Bigg|_{m+1} \left(\rho Y_i|_{m+1} - \rho Y_i|_{m+\frac{1}{2}}\right)\right].$$

Correction

This increases the stability of methods significantly.
However, the pressure stability remains inexact

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An Example Spatially Exact PEP Scheme

A reminder of our two constraints, 3 unknowns:

$$\rho e|_{m+\frac{1}{2}} - \rho e|_m = \sum_{i=1}^{N} \left(\frac{\partial \rho e}{\partial \rho Y_i} \right)_{\rho Y_{j\neq i}, p} \Bigg|_m \left(\rho Y_i|_{m+\frac{1}{2}} - \rho Y_i|_m \right)$$

$$\rho e|_{m+1} - \rho e|_{m+\frac{1}{2}} = \sum_{i=1}^{N} \left(\frac{\partial \rho e}{\partial \rho Y_i} \right)_{\rho Y_{j\neq i}, p} \Bigg|_{m+1} \left(\rho Y_i|_{m+1} - \rho Y_i|_{m+\frac{1}{2}} \right).$$

We let $\rho e|_{m+\frac{1}{2}} = \dfrac{\rho e|_m + \rho e|_{m+1}}{2}.$

Which gives us a 2x2 system to solve for $\rho Y_{1,2}$ at the interface

$$\begin{pmatrix} \epsilon_1|_{m+1} & \epsilon_2|_{m+1} \\ \epsilon_1|_m & \epsilon_2|_m \end{pmatrix} \begin{pmatrix} \rho Y_1|_{m+\frac{1}{2}} \\ \rho Y_2|_{m+\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \rho e|_{m+\frac{1}{2}} - \rho e|_{m+1} + \epsilon_1|_{m+1}\, \rho Y_1|_{m+1} + \epsilon_2|_{m+1}\, \rho Y_2|_{m+1} \\ \rho e|_{m+\frac{1}{2}} - \rho e|_m + \epsilon_1|_m\, \rho Y_1|_m + \epsilon_2|_m\, \rho Y_2|_m \end{pmatrix}.$$

An Example Spatially Exact PEP Scheme

Solving this system will give a spatially exact PEP scheme

$$\begin{pmatrix} \epsilon_1|_{m+1} & \epsilon_2|_{m+1} \\ \epsilon_1|_m & \epsilon_2|_m \end{pmatrix} \begin{pmatrix} \rho Y_1|_{m+\frac{1}{2}} \\ \rho Y_2|_{m+\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \rho e|_{m+\frac{1}{2}} - \rho e|_{m+1} + \epsilon_1|_{m+1}\, \rho Y_1|_{m+1} + \epsilon_2|_{m+1}\, \rho Y_2|_{m+1} \\ \rho e|_{m+\frac{1}{2}} - \rho e|_m + \epsilon_1|_m\, \rho Y_1|_m + \epsilon_2|_m\, \rho Y_2|_m \end{pmatrix}.$$

But it is ill-conditioned as $\left| \epsilon_i|_{m+1} - \epsilon_i|_m \right| \to 0.$

When the left and right state are equal, the arithmetic mean satisfied PEP (No correction is needed)

Proposed PEP Scheme

$$\rho Y_1|^{\text{PEP}}_{m+\frac{1}{2}} = \frac{\rho Y_1|_m + \rho Y_1|_{m+1}}{2} + \alpha,$$

$$\rho Y_2|^{\text{PEP}}_{m+\frac{1}{2}} = \frac{\rho Y_2|_m + \rho Y_2|_{m+1}}{2} - \alpha,$$

$$\rho e|^{\text{PEP}}_{m+\frac{1}{2}} = \frac{\rho e|_m + \rho e|_{m+1}}{2} + \beta - \sum_{i=1}^{N} \left[\frac{\epsilon_i|_{m+1}}{2} \left(\rho Y_i|_{m+1} - \rho Y_i|_{m+\frac{1}{2}} \right) - \frac{\epsilon_i|_m}{2} \left(\rho Y_i|_{m+\frac{1}{2}} - \rho Y_i|_m \right) \right].$$

- Correction parameters should approach 0 in the limit that left and right state are equal
- Preserves the total mass advection
- 2 unknowns, 2 equations
- Free choice of underlying method (APEC in this case)

Numerical Instability of Proposed Scheme

1.) Can use the exact representation and design some switch:

$$\alpha = \frac{\sum_{i=1}^{N}\left(\epsilon_i|_m + \epsilon_i|_{m+1}\right)\left(\rho Y_i|_m - \rho Y_i|_{m+1}\right) + 2\left(\rho e|_{m+1} - \rho e|_m\right)}{2\left[\left(\epsilon_1|_m - \epsilon_1|_{m+1}\right) - \left(\epsilon_2|_m - \epsilon_2|_{m+1}\right)\right]},$$

$$\beta = \frac{\left[\left(\epsilon_1|_m + \epsilon_1|_{m+1}\right) - \left(\epsilon_2|_m + \epsilon_2|_{m+1}\right)\right]\left[\sum_{i=1}^{N}\left(\epsilon_i|_m + \epsilon_i|_{m+1}\right)\left(\rho Y_i|_m - \rho Y_i|_{m+1}\right) - 2\left(\rho e|_m - \rho e|_{m+1}\right)\right]}{4\left[\left(\epsilon_1|_m - \epsilon_1|_{m+1}\right) - \left(\epsilon_2|_m - \epsilon_2|_{m+1}\right)\right]}.$$

2.) Treat it as an ill-conditioned linear algebra problem:

$$\begin{bmatrix} \epsilon_1|_{m+1} - \epsilon_2|_{m+1} & -1 \\ -\epsilon_1|_m + \epsilon_2|_m & 1 \end{bmatrix}\begin{bmatrix}\alpha \\ \beta\end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N}\left[\epsilon_i|_{m+1}\left(-\frac{1}{2}\rho Y_i|_m + \frac{1}{2}\rho Y_i|_{m+1}\right) - \left(-\frac{\epsilon_i|_m}{2} + \frac{\epsilon_i|_{m+1}}{2}\right)\frac{-\rho Y_i|_m + \rho Y_i|_{m+1}}{2}\right] + \frac{1}{2}\left(\rho e|_m - \rho e|_{m+1}\right) \\ \sum_{i=1}^{N}\left[\epsilon_i|_m\left(-\frac{1}{2}\rho Y_i|_m + \frac{1}{2}\rho Y_i|_{m+1}\right) + \left(-\frac{\epsilon_i|_m}{2} + \frac{\epsilon_i|_{m+1}}{2}\right)\frac{-\rho Y_i|_m + \rho Y_i|_{m+1}}{2}\right] + \frac{1}{2}\left(\rho e|_m - \rho e|_{m+1}\right) \end{bmatrix}.$$

Numerical Instability of Proposed Scheme

We'll use the Moore-Penrose pseudo-inverse to solve for α and β.

$$\begin{bmatrix} \epsilon_1|_{m+1} - \epsilon_2|_{m+1} & -1 \\ -\epsilon_1|_m + \epsilon_2|_m & 1 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} \left[\epsilon_i|_{m+1} \left(-\frac{1}{2}\,\rho Y_i|_m + \frac{1}{2}\,\rho Y_i|_{m+1} \right) - \left(-\frac{\epsilon_i|_m}{2} + \frac{\epsilon_i|_{m+1}}{2} \right) \frac{-\rho Y_i|_m + \rho Y_i|_{m+1}}{2} \right] + \frac{1}{2}\left(\rho e|_m - \rho e|_{m+1}\right) \\ \sum_{i=1}^{N} \left[\epsilon_i|_m \left(-\frac{1}{2}\,\rho Y_i|_m + \frac{1}{2}\,\rho Y_i|_{m+1} \right) + \left(-\frac{\epsilon_i|_m}{2} + \frac{\epsilon_i|_{m+1}}{2} \right) \frac{-\rho Y_i|_m + \rho Y_i|_{m+1}}{2} \right] + \frac{1}{2}\left(\rho e|_m - \rho e|_{m+1}\right) \end{bmatrix}.$$

This has a reciprocal condition number hyper-parameter

Reciprocal Condition Number Hyperparameter

- At each timestep, or even each interface, one can choose a new reciprocal condition number to solve the system.
- When the pseudo-inverse zeros the singular values, the scheme reverts to the underlying scheme (APEC)
- We find, that for our problems, it is best to choose a single *safe* estimate



- More accurate
- More likely to run into numerical instability

- Less accurate (more utilization of underlying *approximate* method)
- More numerically stable
- Safer

A Single Reciprocal Condition Number Value

- Step 1: Renormalize A

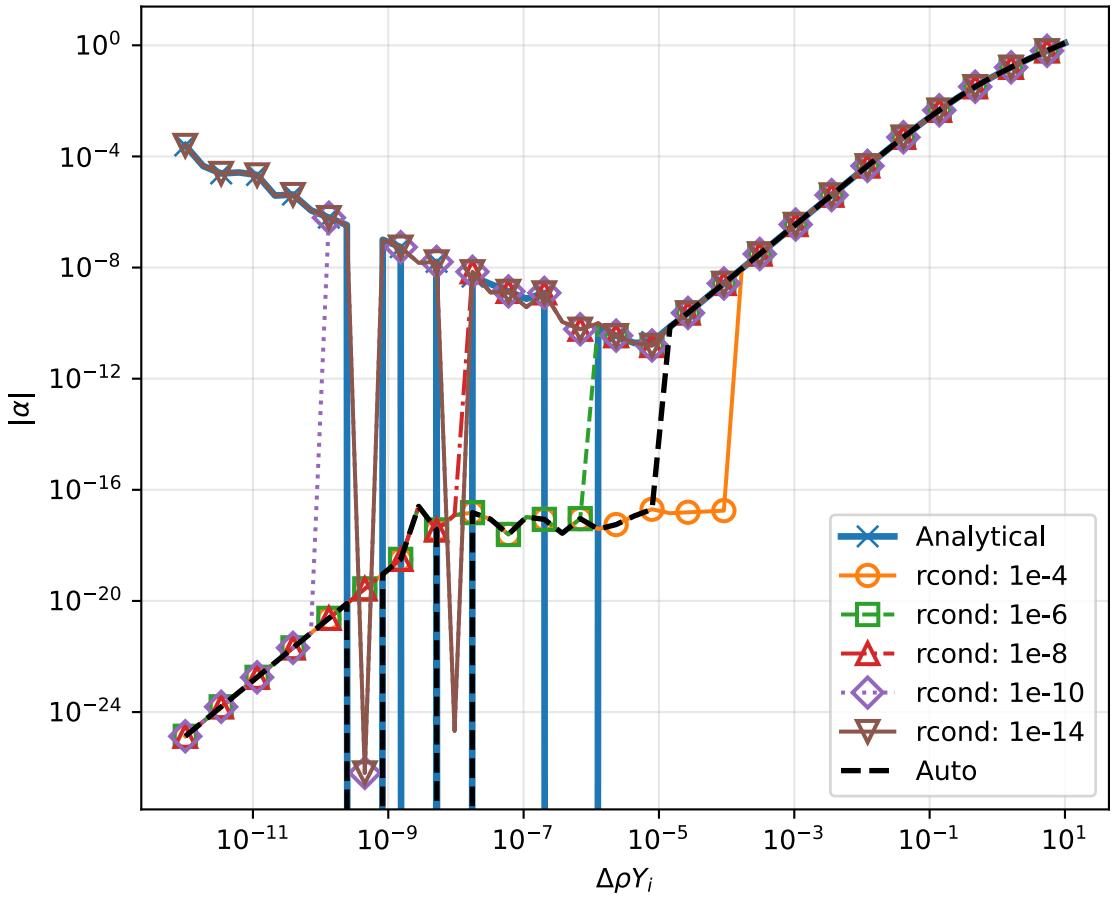
$$\widetilde{A}_{m+\frac{1}{2}} = \begin{bmatrix} \dfrac{\epsilon_1^{m+1} - \epsilon_2^{m+1}}{\sqrt{\max\left(|\epsilon_1^m - \epsilon_2^m|, |\epsilon_1^{m+1} - \epsilon_2^{m+1}|, 1\right)}} & -1 \\ -\dfrac{\epsilon_1^m - \epsilon_2^m}{\sqrt{\max\left(|\epsilon_1^m - \epsilon_2^m|, |\epsilon_1^{m+1} - \epsilon_2^{m+1}|, 1\right)}} & 1 \end{bmatrix}$$

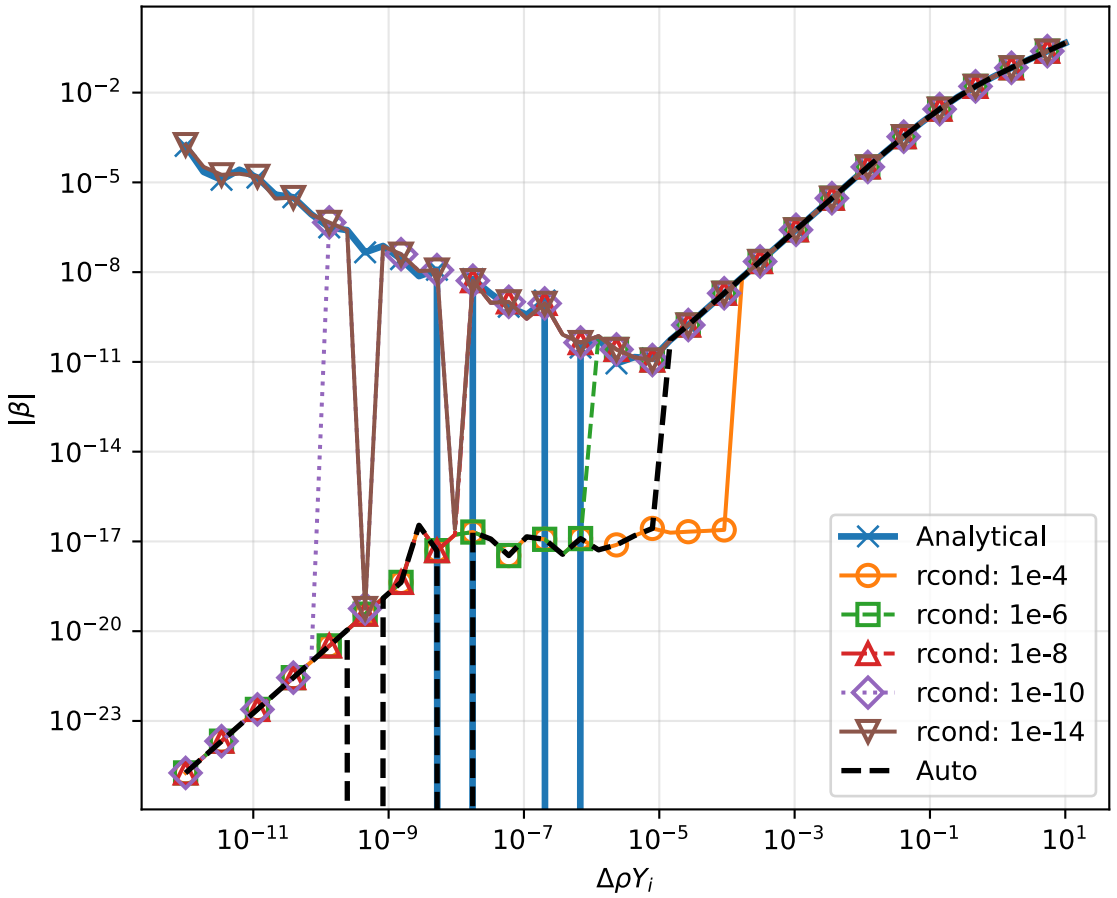
- We solve for eigenvalues of G as a scale independent measure of condition number:

$$G_{m+\frac{1}{2}} \equiv \widetilde{A}^{\top}_{m+\frac{1}{2}} \widetilde{A}_{m+\frac{1}{2}} \qquad r_{m+\frac{1}{2}} = \frac{\lambda_{\min}\left(G_{m+\frac{1}{2}}\right)}{\lambda_{\max}\left(G_{m+\frac{1}{2}}\right)},$$

- At t=0, we take the max over the grid (with some minimum safe-guard) and use this for the entire simulation

Ideal Gas Sensitivity to rcond





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Ideal Gas Test Case

Fluid 1: γ = 1.4, Molecular Weight = 28 g/mol

Fluid 2: γ = 1.66, Molecular Weight = 4 g/mol

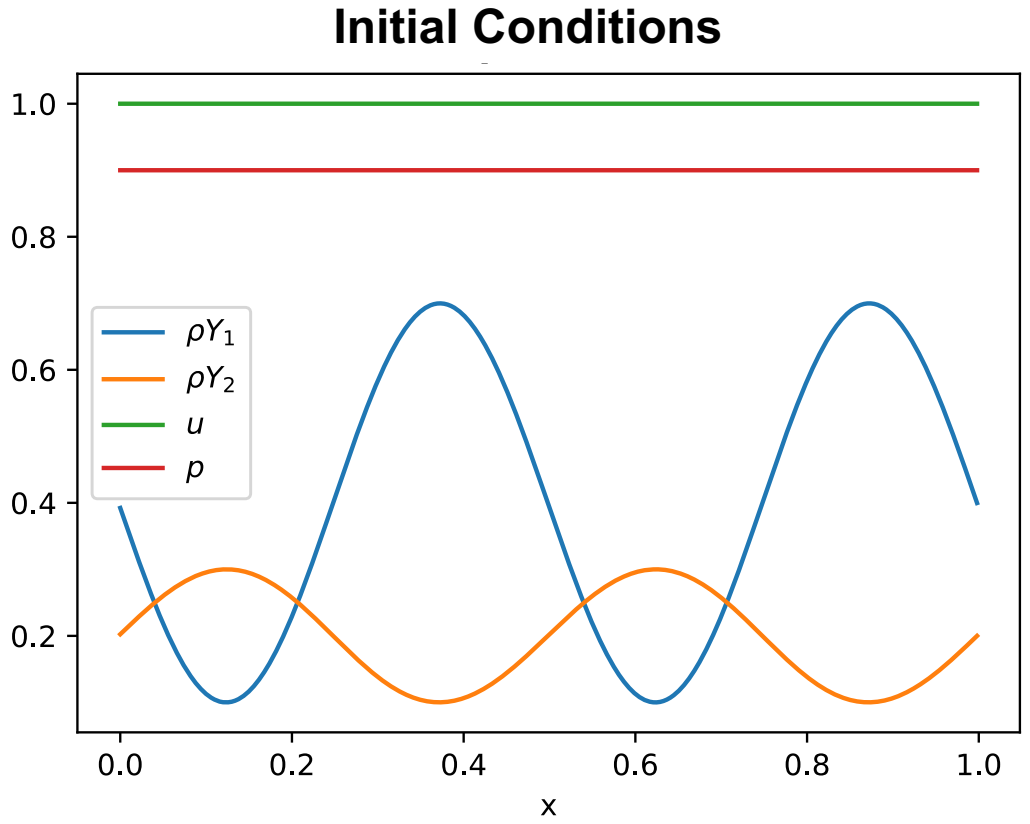
501 cells

4th Order Runge-Kutta

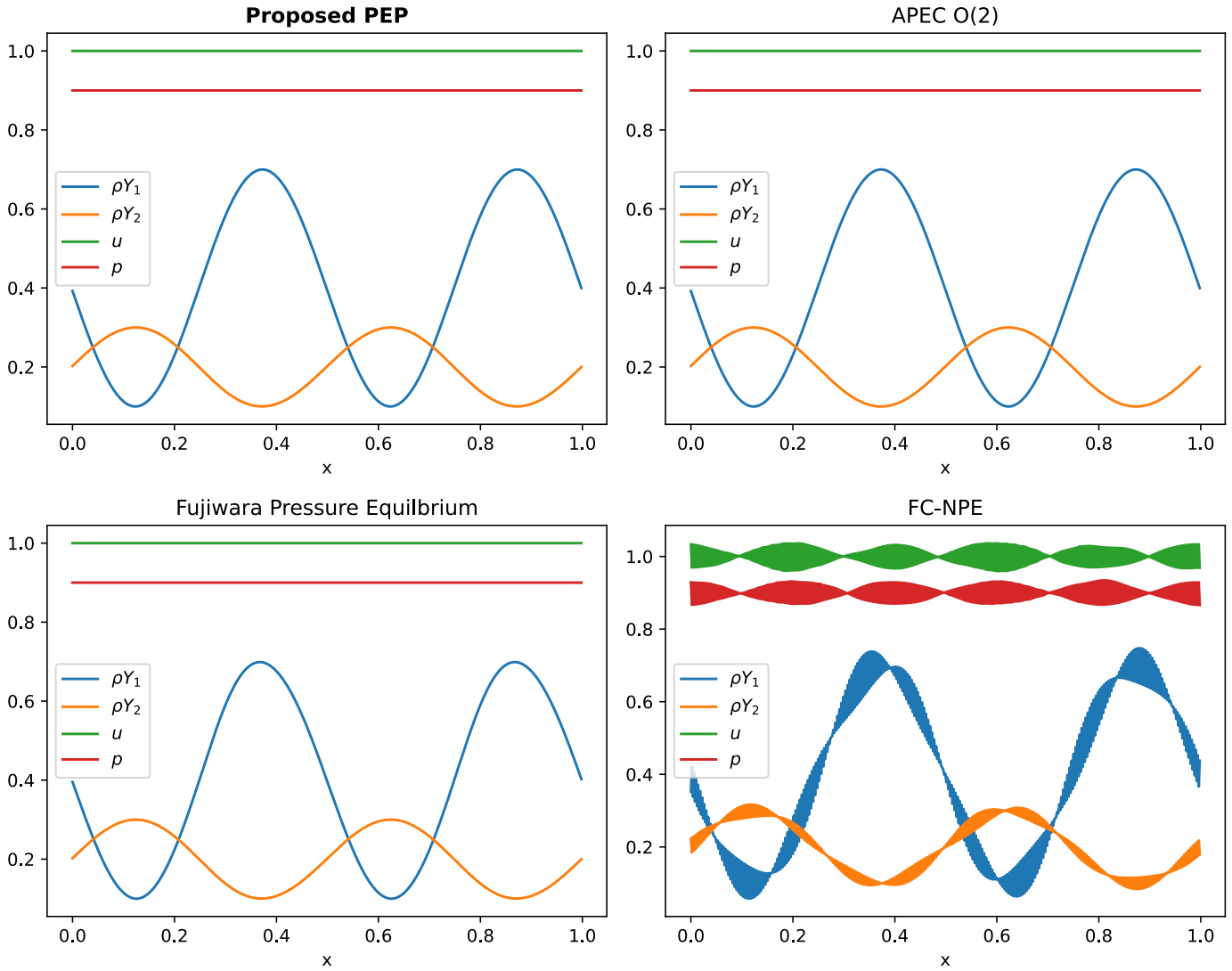
CFL = 0.6

Periodic BCs

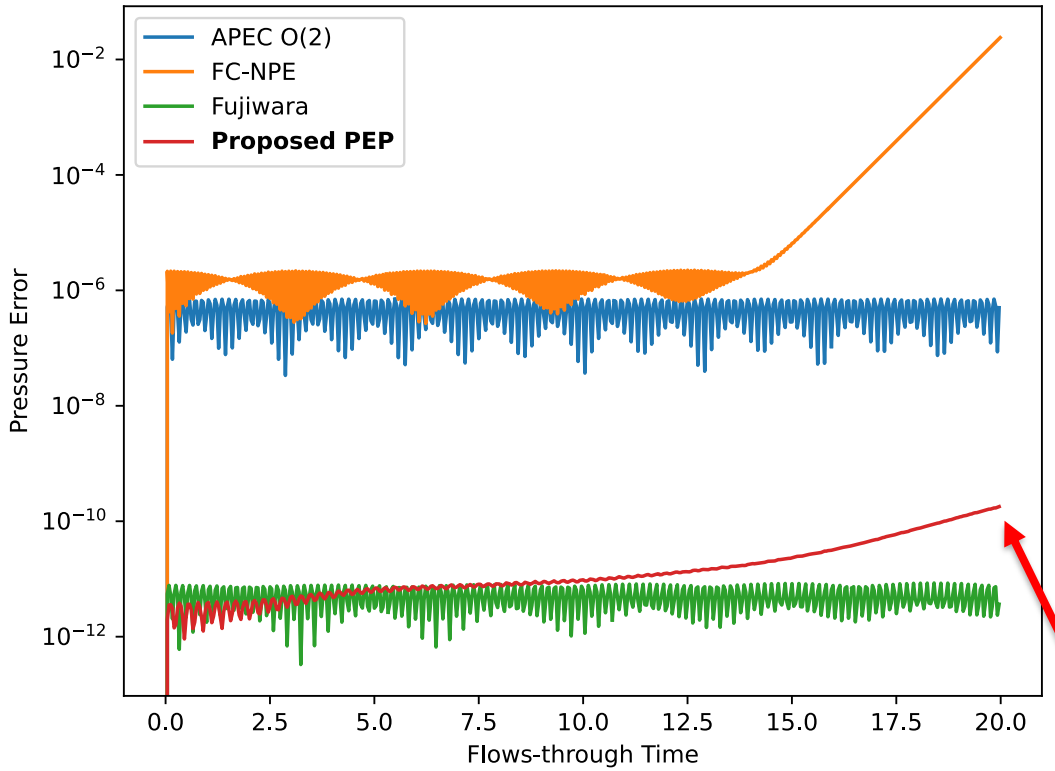
Equation of State: $\rho e = \dfrac{P}{\bar{\gamma} - 1}$

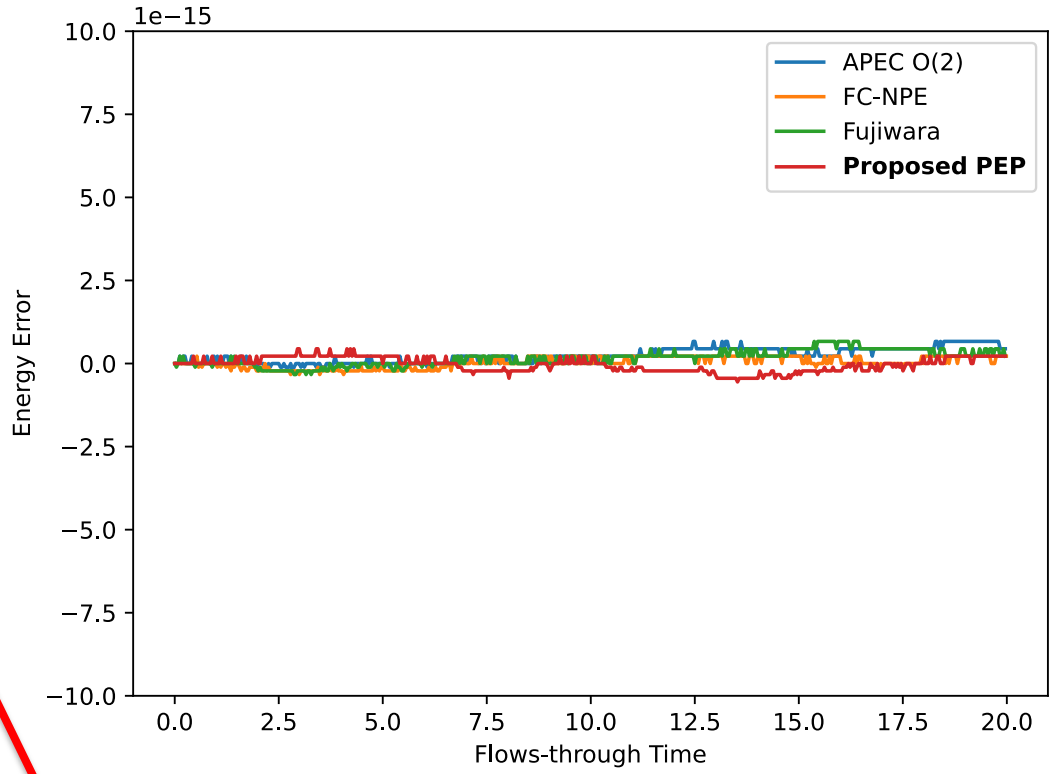


Ideal Gas Test Case at 20 CTUs



Ideal Gas Test Case at 20 CTUs





Increase in pressure error due to pseudo-inverse

Van der Waals Gas Test Case

Fluid 1: γ = 1.4, Molecular Weight = 28 g/mol

T_C = 126.2 K, P_C = 3.39 MPa

Fluid 2: γ = 1.4, Molecular Weight = 32 g/mol

T_C = 154.5 K, P_C = 5.04 MPa

100 cells

4th Order Runge-Kutta

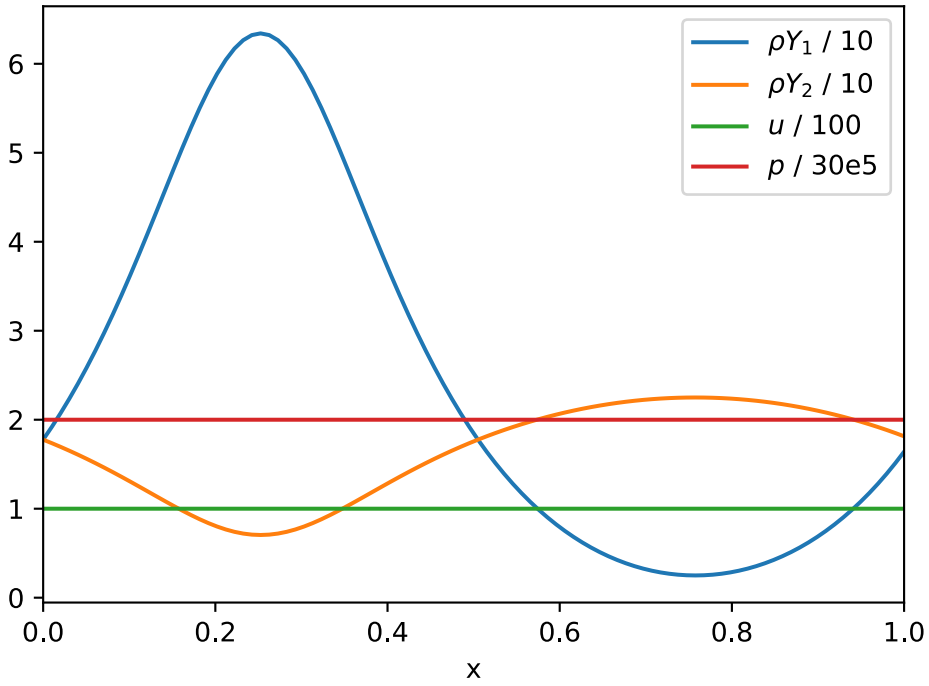
CFL = 0.6

Periodic BCs

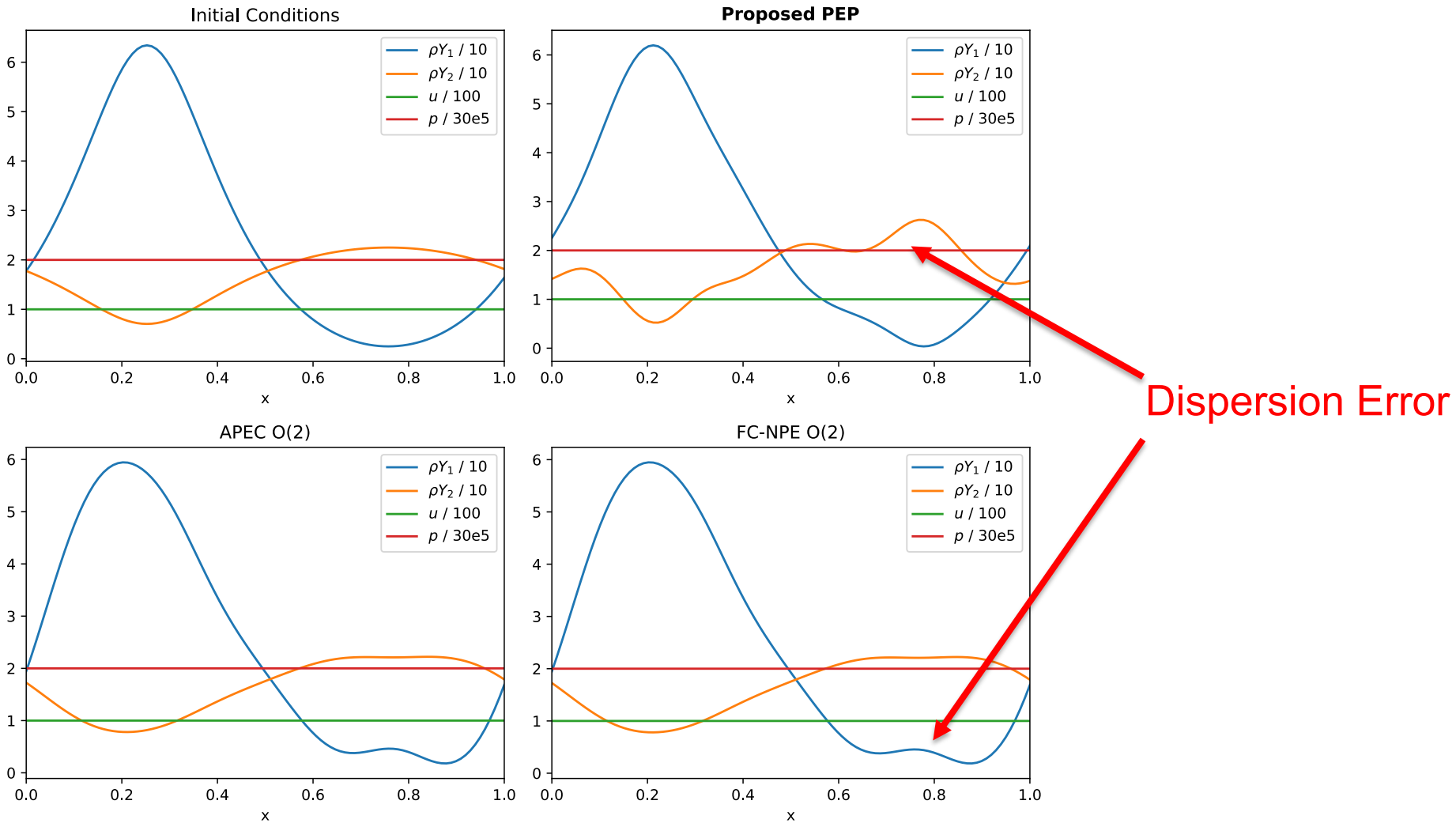
Equation of State: $\left(p + \frac{\bar{a}}{v^2}\right)\left(v - \bar{b}\right) = RT$

$$\begin{pmatrix} Y_{1,0} \\ Y_{2,0} \\ u_0 \\ T_0 \\ p_0 \end{pmatrix} = \begin{pmatrix} 0.4\ \sin(2\pi x) + 0.5 \\ 1 - Y_{1,0} \\ 100 \\ 600 - 300\ \sin(2\pi x) \\ 60 \times 10^5 \end{pmatrix},$$

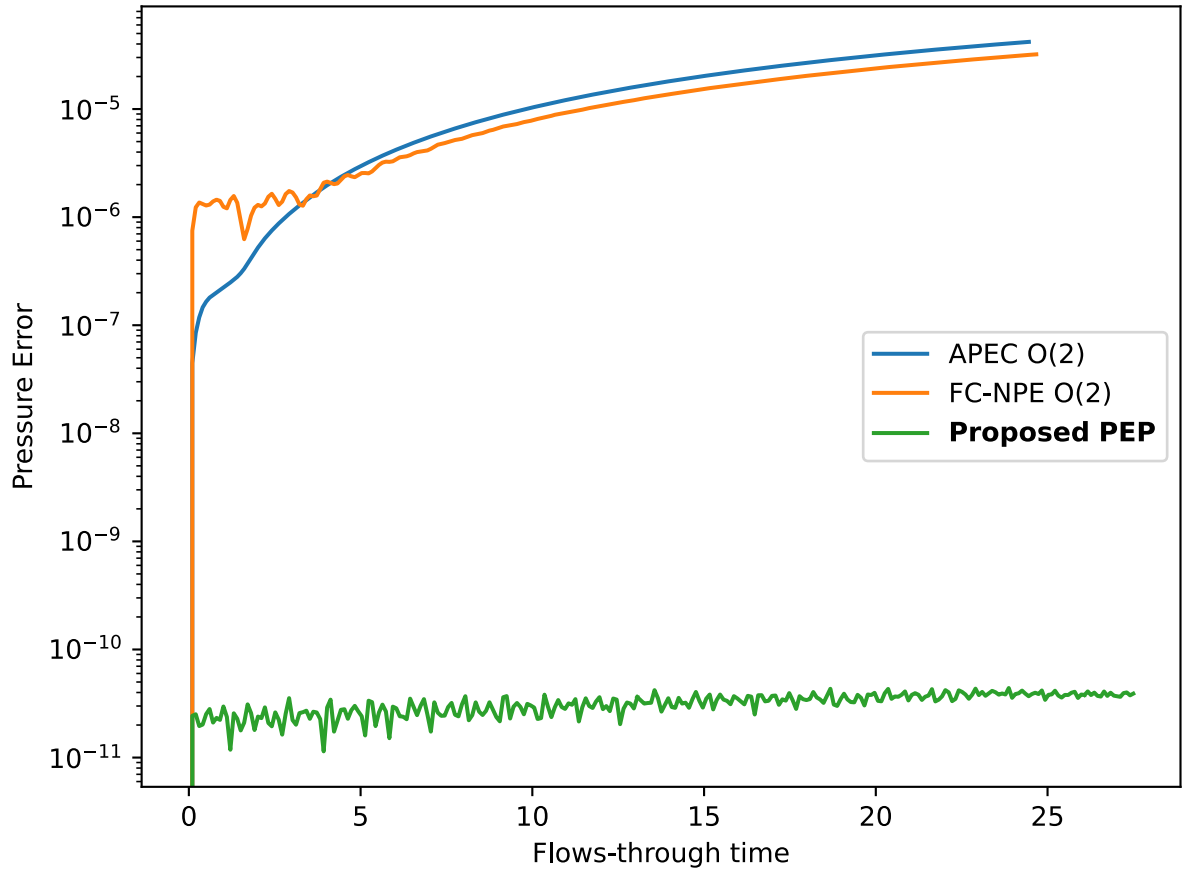
Initial Conditions



Van der Waals Test Case at 20 CTUs



Van der Waals Test Case at 20 CTUs



Outline

Single-species and Multi-species

1. Pressure In-Equilibrium Analysis
2. Spatially Exact PEP Scheme
3. Results

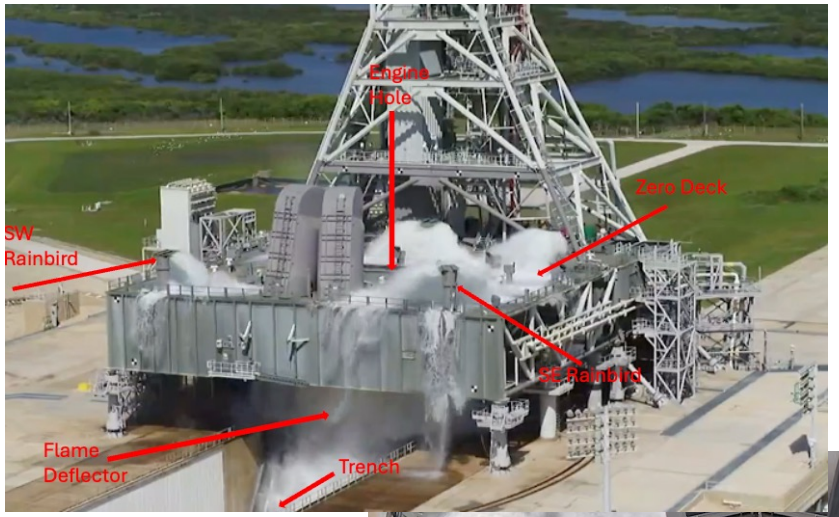
Multi-phase

4. **Augmented 5-Equation Formulation**
5. Extension of PEP Scheme
6. Results

Motivation

- For multiphase configuration involving highly dispersed flows, one appealing strategy is to adopt a volume-averaged method to describe the two-phase mixture

- At NASA, the key application is the modeling of launch-pad acoustic environment under the effects of water-suppression systems



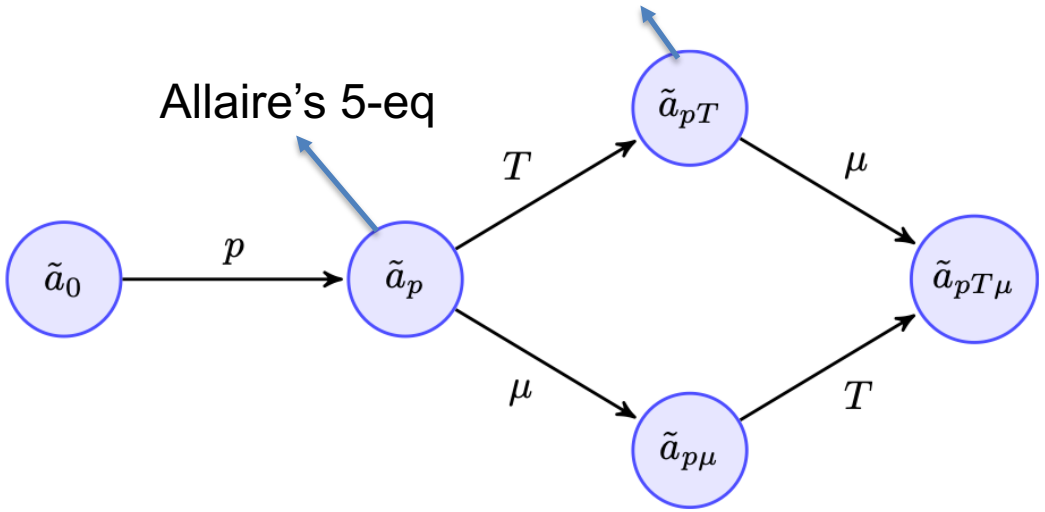


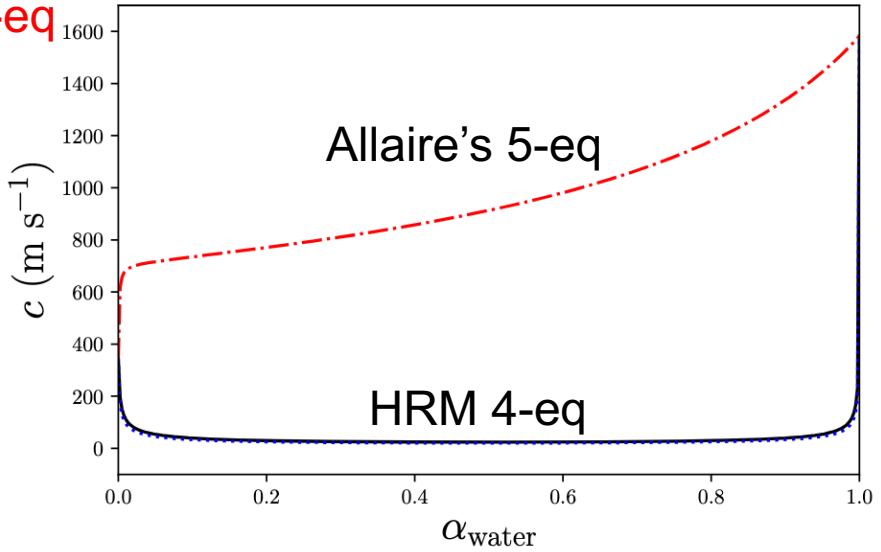
https://images-assets.nasa.gov/video/KSC-20231024-MH-CSH01-0001-Artemis_II_Water_Deluge_Test_39_B-M1718/KSC-20231024-MH-CSH01-0001-Artemis_II_Water_Deluge_Test_39_B-M1718~orig.mp4

Multiphase Approaches in Literature

- Eulerian-Eulerian multiphase models can be constructed via a hierarchy of phase interactions (Flatten & Lund 2012)
  - Each with a different mixture acoustic-wave speed

Homogeneous Relaxation Model (HRM) 4-eq





- There are two main challenges with the numerical solution of Eulerian-Eulerian multiphase models with p-T relaxation:
  - Challenge 1: HRM 4-eq models lead to very low sound-speed in the dispersed-phase region
    => reduced dissipation in approximate Riemann solvers
  - Challenge 2: Maintaining pressure-equilibrium(PEQ) property is not yet achieved

PEQ property:

At t_n: $p(x) = p_0, u(x) = u_0$ with arbitrary temperature and composition profiles

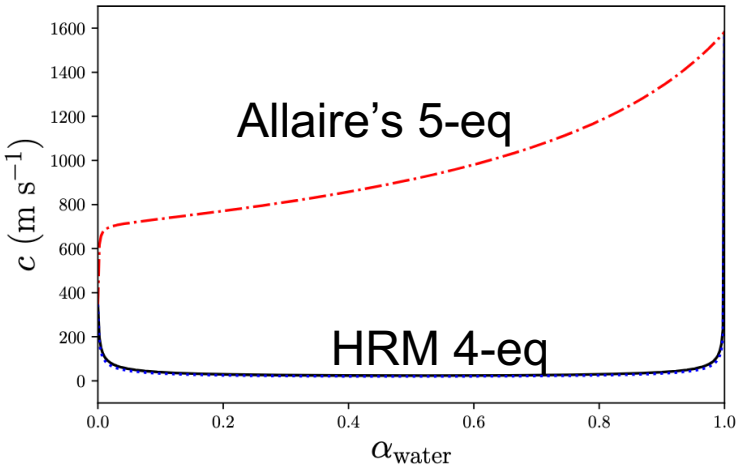
At t_{n+1}: $p(x) = p_0, u(x) = u_0$

Our Past Approach

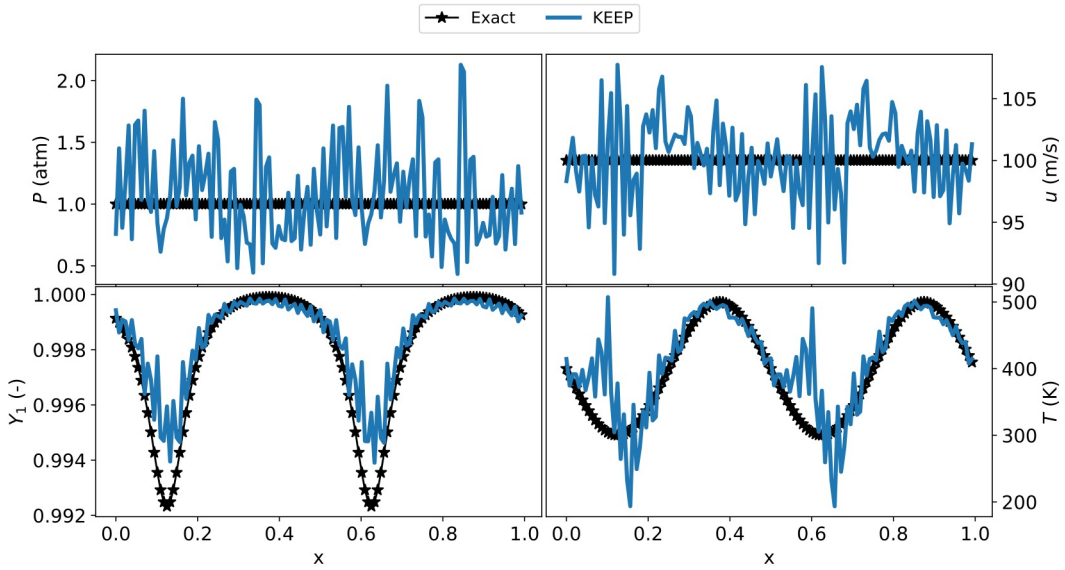
- For the numerical solution of the HRM 4-eq model, we have overcome Challenge 1 and *partially* overcome Challenge 2

- The solution for challenge 1 is via a split-step approach:
  - Hyperbolic step with Allaire's 5-eq model
  - Algebraic temperature relaxation step between the phases

  - Then, the sound-speed in the hyperbolic step is monotonic w.r.t. volume fraction



- This only *partially solves Challenge 2* since Allaire's 5-eq model only guarantees PEQ for constant temperature profiles



Mathematical Model

- Hyperbolic Step: Allaire's 5-eq model:

Partial densities
$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial(\rho Y_k u)}{\partial x} = 0,$$

Momentum
$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u u + p)}{\partial x} = 0,$$

Energy
$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial\left[(\rho E + p)u\right]}{\partial x} = 0,$$

Volume fraction
$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = 0,$$

- Temperature-relaxation step:

$$\frac{\partial(\rho Y_k)}{\partial t} = 0, \quad \frac{\partial(\rho u)}{\partial t} = 0, \quad \frac{\partial(\rho E)}{\partial t} = 0, \quad \frac{\partial \phi}{\partial t} = H(T_1 - T_2),$$

	Water	Air
p_∞	1e9	0
q	-1.167e6	0
c_v	1816	719.3
γ	2.35	1.4

- Stiffened-gas mixture EOS model:

$$\rho = \sum_{k=1}^{2} \phi_i \rho_i = \sum_{k=1}^{2} \rho Y_i, \quad \rho e = \sum_{k=1}^{2} \phi_k \rho_k e_k. \qquad \frac{p_k}{(\gamma_k - 1)} + \frac{\gamma_k p_k^\infty}{(\gamma_k - 1)} = \rho_k(e_k - q_k), \quad \text{and} \quad T_k = \frac{(p_k + p_k^\infty)}{\left[(\gamma_k - 1)\rho_k c_{v,k}\right]},$$

Outline

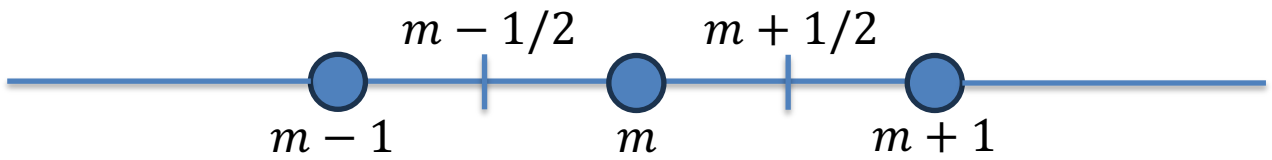
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Derivation of PEQ Criterion



- We consider a method of lines for the hyperbolic step
  - With KEEP form for the discretized convective fluxes (Kuya & Kawai, 2020)

$$\left.\frac{d(\rho Y_1)}{dt}\right|_m + F_{\rho Y_1}|_m = 0$$
$$\left.\frac{d(\rho Y_2)}{dt}\right|_m + F_{\rho Y_2}|_m = 0$$
$$\left.\frac{d(\rho u)}{dt}\right|_m + F_{\rho u}|_m = 0$$
$$\left.\frac{\partial(\rho E)}{\partial t}\right|_m + F_{\rho E}|_m = 0$$
$$\left.\frac{d\phi}{dt}\right|_m + F_{\phi}|_m = 0$$

$$F_{\rho Y_1}|_m = \frac{C_1|_{m+\frac{1}{2}} - C_1|_{m-\frac{1}{2}}}{\Delta x}$$
$$F_{\rho Y_2}|_m = \frac{C_2|_{m+\frac{1}{2}} - C_2|_{m-\frac{1}{2}}}{\Delta x}$$
$$F_{\rho u}|_m = \frac{M|_{m+\frac{1}{2}} - M|_{m-\frac{1}{2}}}{\Delta x} + \frac{\Pi|_{m+\frac{1}{2}} - \Pi|_{m-\frac{1}{2}}}{\Delta x}$$
$$F_{\rho E}|_m = \frac{K|_{m+\frac{1}{2}} - K|_{m-\frac{1}{2}}}{\Delta x} + \frac{I|_{m+\frac{1}{2}} - I|_{m-\frac{1}{2}}}{\Delta x} + \frac{S|_{m+\frac{1}{2}} - S|_{m-\frac{1}{2}}}{\Delta x},$$

$$C_1|_{m+\frac{1}{2}} = \rho Y_1|_{m+\frac{1}{2}} \frac{u|_m + u|_{m+1}}{2}$$
$$C_2|_{m+\frac{1}{2}} = \rho Y_2|_{m+\frac{1}{2}} \frac{u|_m + u|_{m+1}}{2}$$
$$M|_{m+\frac{1}{2}} = \rho|_{m+\frac{1}{2}} \frac{u|_m + u|_{m+1}}{2} \frac{u|_m + u|_{m+1}}{2}$$
$$\Pi|_{m+\frac{1}{2}} = \frac{p|_m + p|_{m+1}}{2}$$
$$K|_{m+\frac{1}{2}} = \rho|_{m+\frac{1}{2}} \frac{u|_m + u|_{m+1}}{2} \frac{u|_m\, u|_{m+1}}{2}$$
$$I|_{m+\frac{1}{2}} = \rho e|_{m+\frac{1}{2}} \frac{u|_m + u|_{m+1}}{2}$$
$$S|_{m+\frac{1}{2}} = \frac{u|_m\, p|_{m+1} + u|_{m+1}\, p|_m}{2}$$

- The volume fraction transport also follows a KEEP form

$$\left.\frac{\partial \phi}{\partial t}\right|_m + \frac{\phi|_{m+\frac{1}{2}}\, u|_{m+\frac{1}{2}} - \phi|_{m-\frac{1}{2}}\, u|_{m-\frac{1}{2}}}{\Delta x} - \phi|_m \frac{u|_{m+\frac{1}{2}} - u|_{m-\frac{1}{2}}}{\Delta x} = 0.$$

Derivation of PEQ Criterion (cont.)

- The problem is to maintain pressure-equilibrium through the hyperbolic split-step + relaxation split-step:

Define the choice of mid-point values $\rho Y_1|_{m+\frac{1}{2}}, \rho Y_2|_{m+\frac{1}{2}}, \rho|_{m+\frac{1}{2}}, \phi|_{m+\frac{1}{2}}, \rho e|_{m+\frac{1}{2}}$

such that for one step of the hyperbolic split-step

$$\text{If} \quad \begin{cases} u|_m^n = U_0 \\ p|_m^n = p_0 \\ T_1|_m^n = T_2|_m^n \end{cases} \quad \text{then} \quad \begin{cases} u|_m^{n+1} = U_0 \\ p|_m^{n+1} = p_0 \\ T_1|_m^{n+1} = T_2|_m^{n+1} \end{cases}$$

Maintains PEQ through relaxation split-step

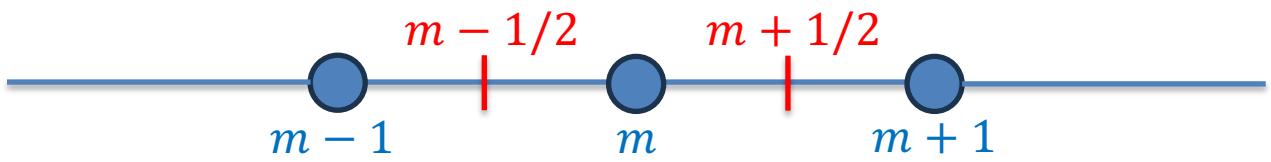
- Approach: Expand the balanced primitives w.r.t. conservative variables
- For example: Velocity equilibrium condition

$$u|_m^{n+1} - u|_m^n = \left(\frac{\partial u}{\partial \rho u}\right)_\rho \Big|_m^n (\rho u|_m^{n+1} - \rho u|_m^n) + \left(\frac{\partial u}{\partial \rho}\right)_{\rho u} \Big|_m^n (\rho|_m^{n+1} - \rho|_m^n) + \text{H.O.}$$

  - This condition is automatically satisfied (to first order in time) if

$$\rho|_{m+\frac{1}{2}} \equiv \rho Y_1|_{m+\frac{1}{2}} + \rho Y_2|_{m+\frac{1}{2}},$$

Derivation of PEQ Criterion (cont.)



- Extending the analysis now to the update rule for pressure and phasic temperature difference, we obtain the criteria for pressure and phasic temperature equilibria (to first-order in time)

$$\left(\rho e|_{m+\frac{1}{2}} - \rho e|_{m-\frac{1}{2}}\right) - \epsilon_{\rho Y_1}|_m \left(\rho Y_1|_{m+\frac{1}{2}} - \rho Y_1|_{m-\frac{1}{2}}\right) - \epsilon_{\rho Y_2}|_m \left(\rho Y_2|_{m+\frac{1}{2}} - \rho Y_2|_{m-\frac{1}{2}}\right) - \epsilon_{\phi}|_m \left(\phi|_{m+\frac{1}{2}} - \phi|_{m-\frac{1}{2}}\right) = 0,$$

$$\beta_{\rho e}|_m \left(\rho e|_{m+\frac{1}{2}} - \rho e|_{m-\frac{1}{2}}\right) + \beta_{\rho Y_1}|_m \left(\rho Y_1|_{m+\frac{1}{2}} - \rho Y_1|_{m-\frac{1}{2}}\right) + \beta_{\rho Y_2}|_m \left(\rho Y_2|_{m+\frac{1}{2}} - \rho Y_2|_{m-\frac{1}{2}}\right) + \beta_{\phi}|_m \left(\phi|_{m+\frac{1}{2}} - \phi|_{m-\frac{1}{2}}\right) = 0.$$

- With the thermodynamic sensitivity variables

$$\epsilon_\Phi \equiv \partial(\rho e)/\partial\Phi \quad \text{and} \quad \beta_\Phi \equiv \partial\Delta T/\partial\Phi$$

defined on the thermodynamic manifolds

$$\rho e(\rho Y_1, \rho Y_2, \phi, p) \text{ and } \Delta T(\rho Y_1, \rho Y_2, \rho e, \phi)$$

- In this current form, there is a telescopic coupling between the nodes

Pressure-Equilibrium Preserving (PEP) Scheme

- After some manipulation, the criteria can be split into local conditions to solve for the mid-point values

$$\mathbf{f}|_{m+\frac{1}{2}} \equiv \left[\rho Y_1|_{m+\frac{1}{2}} \;\; \rho Y_2|_{m+\frac{1}{2}} \;\; \phi|_{m+\frac{1}{2}} \;\; \rho e|_{m+\frac{1}{2}}\right]^T$$

- However, the conditions are *singular* when cells m and $m+1$ are identical
- The solution is to first split up the midpoint values into a base-scheme contribution and a PEP-correction contribution

$$\mathbf{f}|_{m+\frac{1}{2}} = \mathbf{f^0}|_{m+\frac{1}{2}} + \mathbf{c}|_{m+\frac{1}{2}}$$

- Then, the final system to solve for the PEP scheme is

$$\mathbf{A}|_{m+\frac{1}{2}} \; \mathbf{c}|_{m+\frac{1}{2}} = \mathbf{b}|_{m+\frac{1}{2}} - \mathbf{A}|_{m+\frac{1}{2}} \; \mathbf{f^0}|_{m+\frac{1}{2}}$$

$$\mathbf{A}|_{m+\frac{1}{2}} = \begin{pmatrix} -\epsilon_{\rho Y_1}|_m & -\epsilon_{\rho Y_2}|_m & -\epsilon_{\phi}|_m & 1 \\ -\epsilon_{\rho Y_1}|_{m+1} & -\epsilon_{\rho Y_2}|_{m+1} & -\epsilon_{\phi}|_{m+1} & 1 \\ \beta_{\rho Y_1}|_m & \beta_{\rho Y_2}|_m & \beta_{\phi}|_m & \beta_{\rho e}|_m \\ \beta_{\rho Y_1}|_{m+1} & \beta_{\rho Y_2}|_{m+1} & \beta_{\phi}|_{m+1} & \beta_{\rho e}|_{m+1} \end{pmatrix},$$

$$\mathbf{b}|_{m+\frac{1}{2}} = \begin{pmatrix} \rho e|_m - \epsilon_{\rho Y_1}|_m \, \rho Y_1|_m - \epsilon_{\rho Y_2}|_m \, \rho Y_2|_m - \epsilon_{\phi}|_m \, \phi|_m \\ \rho e|_{m+1} - \epsilon_{\rho Y_1}|_{m+1} \, \rho Y_1|_{m+1} - \epsilon_{\rho Y_2}|_{m+1} \, \rho Y_2|_{m+1} - \epsilon_{\phi}|_{m+1} \, \phi|_{m+1} \\ \beta_{\rho e}|_m \, \rho e|_m + \beta_{\rho Y_1}|_m \, \rho Y_1|_m + \beta_{\rho Y_2}|_m \, \rho Y_2|_m + \beta_{\phi}|_m \, \phi|_m \\ \beta_{\rho e}|_{m+1} \, \rho e|_{m+1} + \beta_{\rho Y_1}|_{m+1} \, \rho Y_1|_{m+1} + \beta_{\rho Y_2}|_{m+1} \, \rho Y_2|_{m+1} + \beta_{\phi}|_{m+1} \, \phi|_{m+1} \end{pmatrix}$$

- We solve using pseudo-inverse to correctly relax $\mathbf{c}|_{m+\frac{1}{2}}$ to $\mathbf{0}$ at (near-)singular conditions.

Outline

Single-species and Multi-species

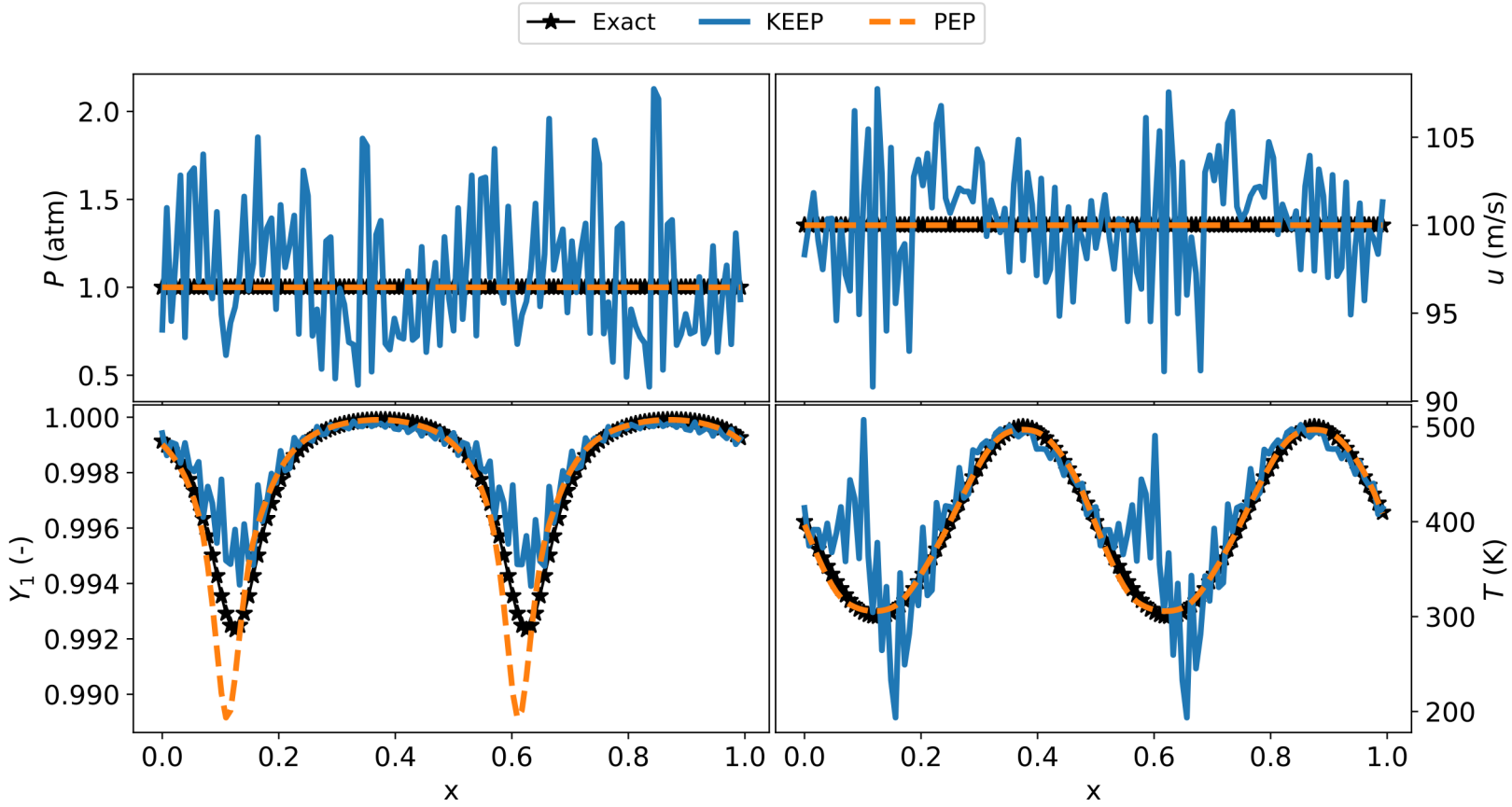
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One-dimensional Advection Test

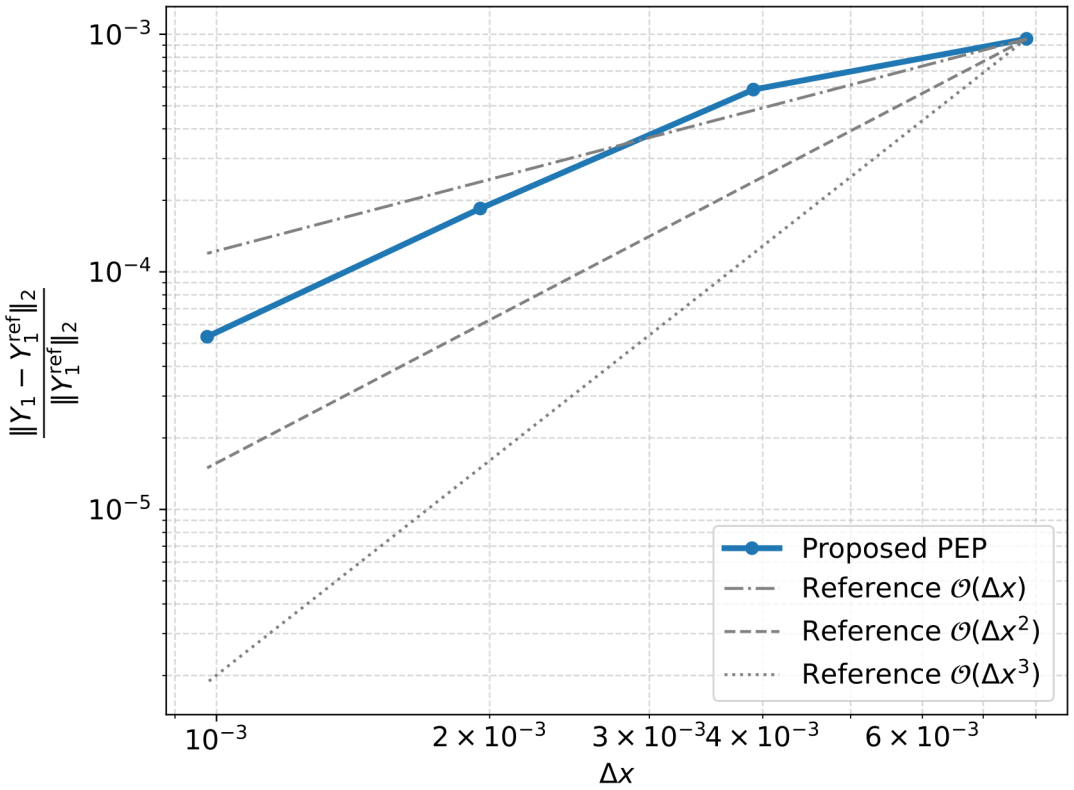
- Water/air mixture with sinusoidal initial profiles.
- SSPRK33 time-stepping scheme. 128-cell grid with domain [0,1] m.
- Showing solution at three flow-through-times (FTTs)
- Standard KEEP scheme results in large pressure/velocity fluctuations that destroy the advected profiles.
- **PEP scheme perfectly preserves pressure and velocity equilibria.**



One-dimensional Advection Test

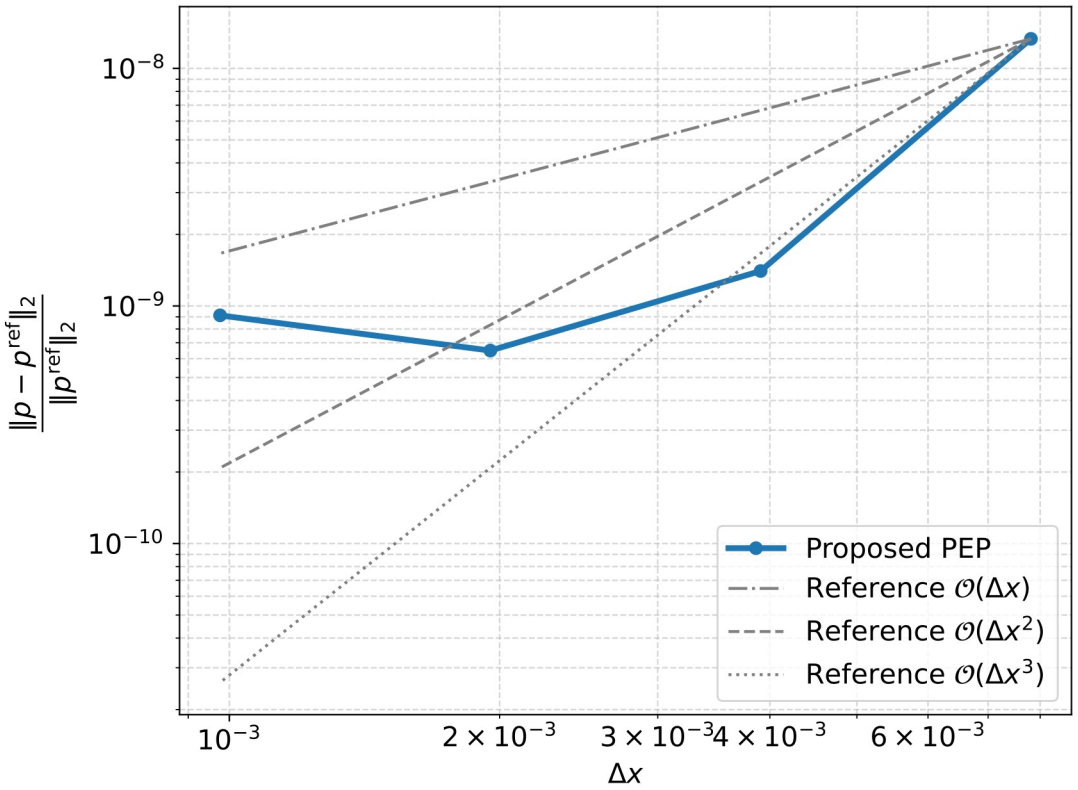
- Convergence analysis:

Water mass-fraction



PEP scheme converges advected profiles like the underlying KEEP scheme (2nd order)

Pressure



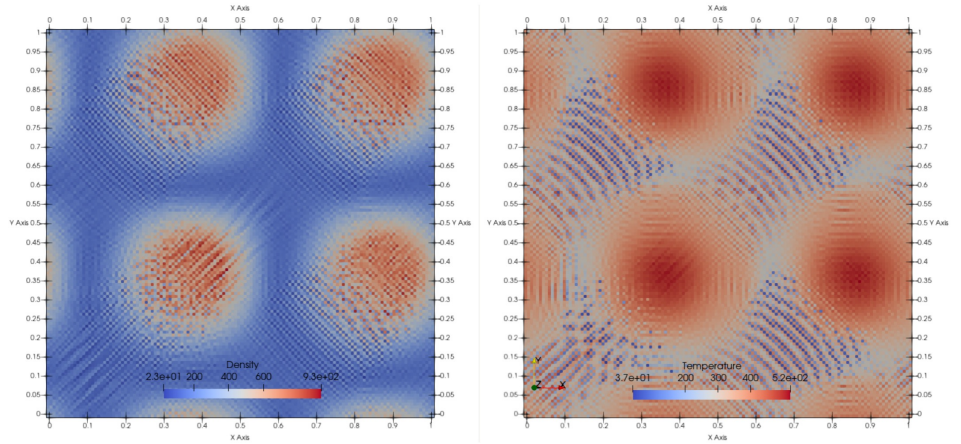
PEP scheme converges pressure equilibrium like the time-stepping scheme (3rd order)

Two-dimensional Advection Test

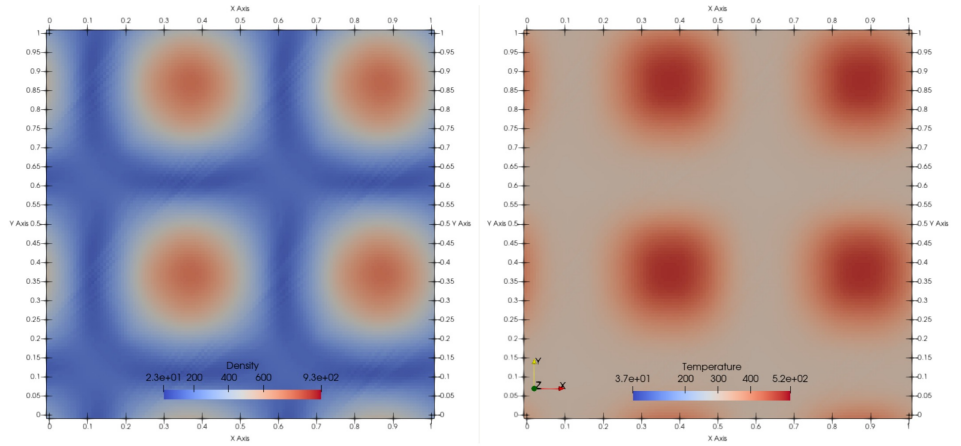
- Water/air mixture with 2D sinusoidal initial profiles, advected diagonally
- SSPRK33 time-stepping scheme. 128x128-cell grid.

- Showing solution at three FTT
- Standard KEEP scheme results in large fluctuations in pressure and velocity
- **PEP scheme perfectly preserves pressure and velocity equilibria.**

Density and temperature fields

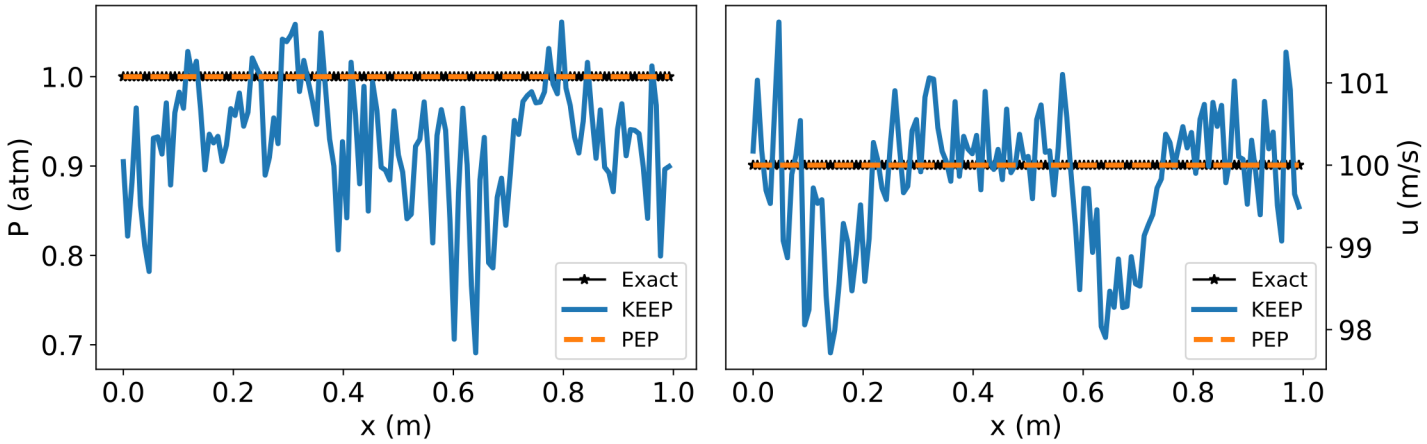


(a) KEEP



(b) PEP

Pressure/velocity profiles



Line probe at constant y

Current Development: Shock Capturing

- The proposed PEP scheme is perfect at maintaining pressure/velocity equilibria.
- However, it remains unsuitable for general flow configurations:
  - The PEP correction is strictly not valid when initial pressure/velocity are in non-equilibrium.
  - The PEP construction is based on the KEEP scheme, thus is not shock capturing.

- Current approach:
  - For generic non-equilibrium flows: Apply an activation to the correction term in the PEP scheme
  - For shock capturing: Blend the PEP scheme with an approximate Riemann solver (e.g. HLLEC)

$$\mathbf{f}|_{m+\frac{1}{2}} = (\mathbf{f}_{\mathrm{KEEP}}|_{m+\frac{1}{2}} + \alpha\, \mathbf{c}|_{m+\frac{1}{2}})$$

WENO shock sensor

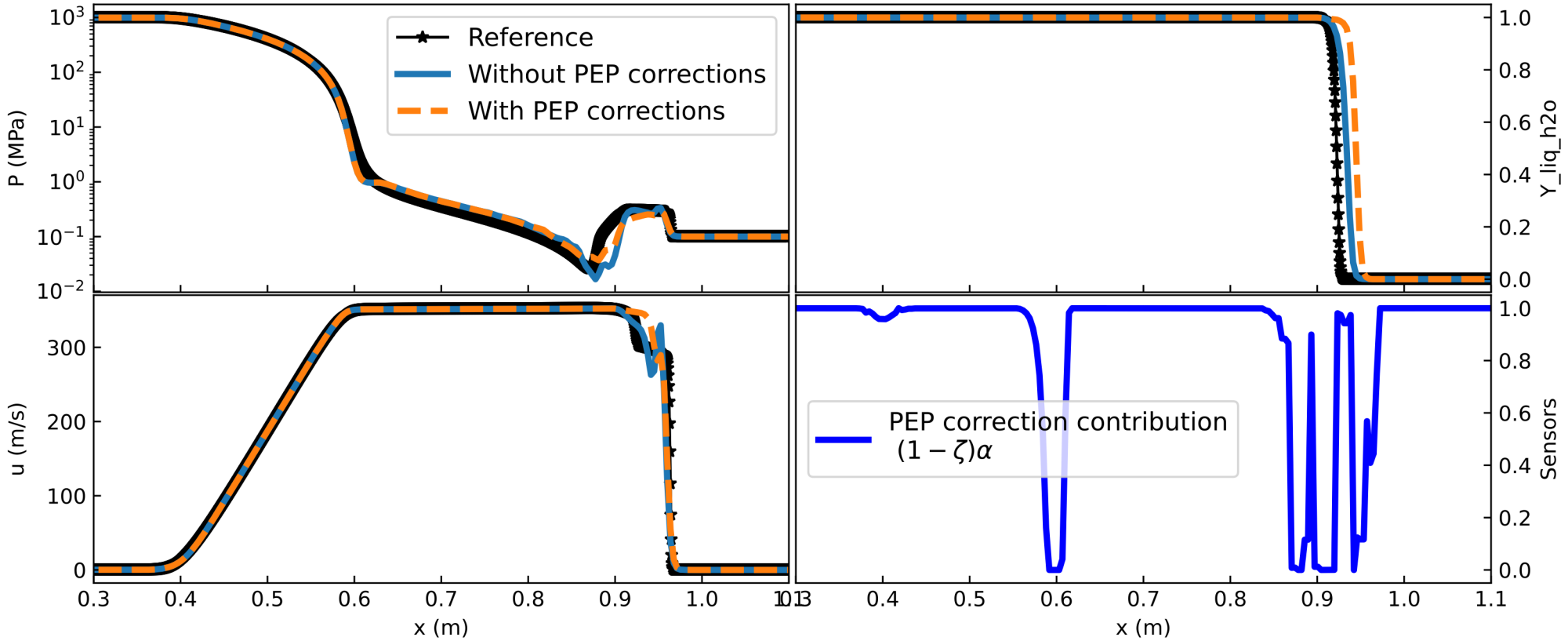
PEP-correction activation sensor
Based on cell-to-cell pressure/velocity differences

Test Case: Two-phase Sod Shock Tube

- Initial condition with pressure and compositional jump.
- SSPRK33 time-stepping, 400-cell grid on domain [0,1.6] m.

$$[p, u, Y_{\text{liq}}, T] = \begin{cases} [10^9 \text{ Pa}, 0, 1, 300 \text{ K}] \text{ if } x < 0.8 \text{ m} \\ [10^5 \text{ Pa}, 0, 0, 300 \text{ K}] \text{ if } x > 0.8 \text{ m} \end{cases}$$

- Showing solution at $t = 30$ ms
- Hybrid KEEP/HLLEC scheme successfully capture the shock.
- **Adding in PEP corrections eliminates velocity fluctuations just behind the shock.**

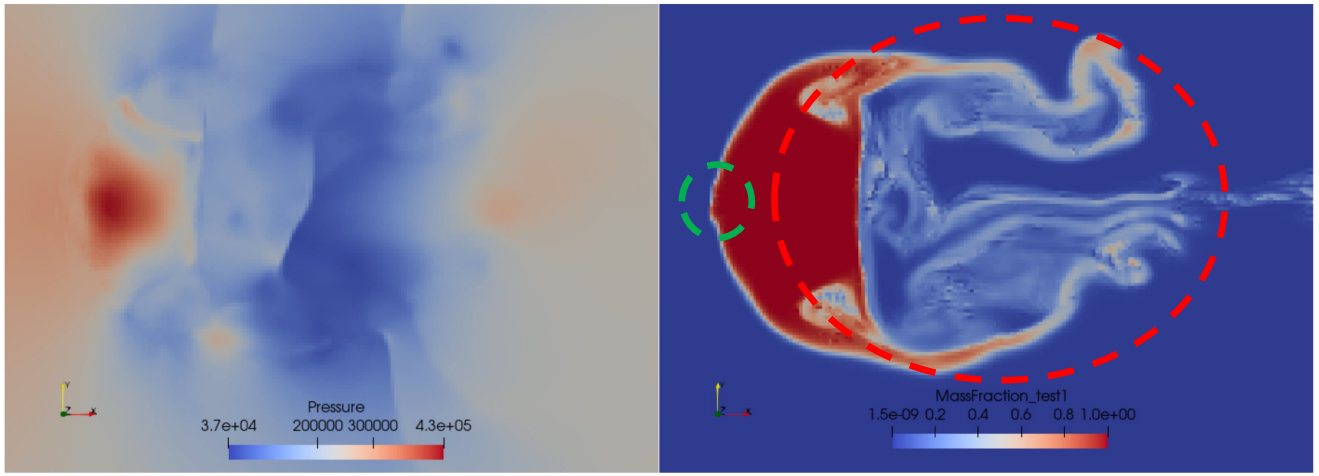


Test Case: Shock/Water-column interaction

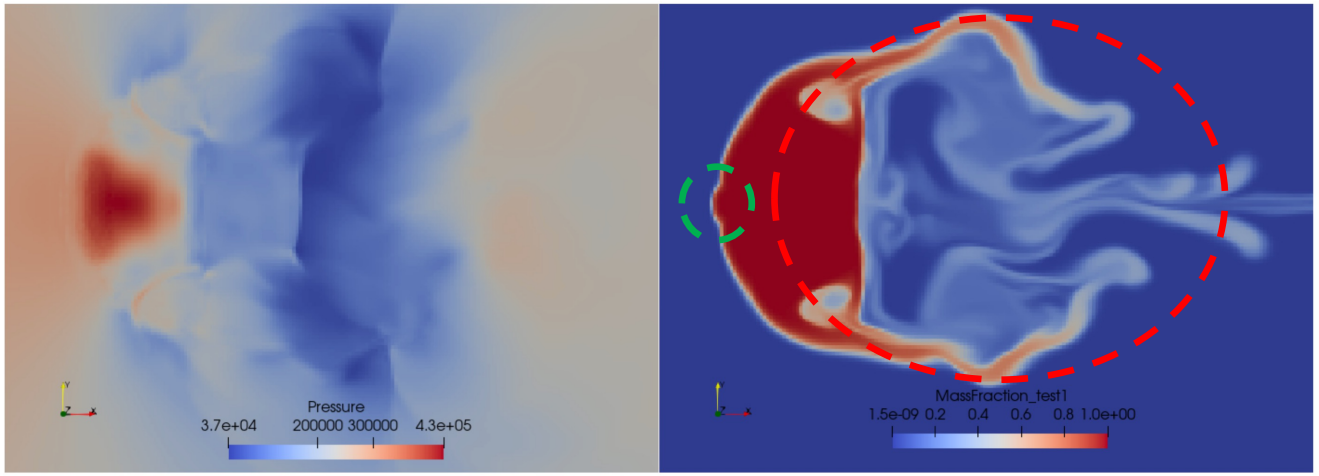
- Initial condition: Mach 1.47 shock wave in air ahead of a water column with D = 4.8 mm at room conditions
- SSPRK33 time-stepping, 50 cells per column diameter

- Showing solution at $t = 146\ \mu s$
- Hybrid KEEP/HLLEC scheme successfully capture the shock without robustness issue.
- **Adding in PEP corrections slightly improves the smoothness of the column leading edge**
- **However, significant numerical artifacts observed in the wake due to incorrect activation of PEP corrections**

Pressure | Liquid mass-fraction



(a) With PEP corrections



(b) Without PEP corrections

Conclusion

We introduce a construction recipe for Exact Pressure-Equilbrium-Preserving Scheme:

Properties:

- Fully Conservative
- Compatible with an arbitrary EOS
- Free choice of underlying discretization method
  - In this work we use KEEP, but these methods can be easily applied to any numerical flux formulation
- Show orders of magnitude decreases in pressure error

The construction applies to:

- Four-equation multispecies Euler equation
- Five-equation multiphase Euler equation with temperature relaxation

Ongoing Challenges:

- Key limitation: central PEP flux lacks dissipation for shocks and offers no stability guarantee away from pressure/velocity equilibrium
- Proposed fix: hybrid blending of central PEP with dissipative HLLEC Riemann solver, gated by a sensor restricting PEP corrections to near-equilibrium regions
- Proof-of-concept shows some limited improved robustness across shock cases
  - Robustness issues remains from activating PEP corrections in regions of non-equilibrium.
- Ongoing work: refining the blending/sensor strategy for robust shock-interface coupling

References and Acknowledgements

- Fully conservative and pressure-equilibrium preserving scheme for compressible multi-component flows (Fujiwara et al., 2023)
- Approximately pressure-equilibrium-preserving scheme for fully conservative simulations of compressible multi-species and real-fluid interfacial flows (Terashima et al., 2025)
- High-order accurate kinetic-energy and entropy preserving (KEEP) schemes on curvilinear grids (Kuya et al., 2021)
- **On the Construction of High-Order and Exact Pressure Equilibrium Schemes for Arbitrary Equations of State (DeGrendele et al., 2025)**
- **Construction of an Exact Pressure-Equilibrium Scheme for the Five-Equation Two-Phase Flow Model with Thermal Relaxation (Ly et al., 2026)**

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