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

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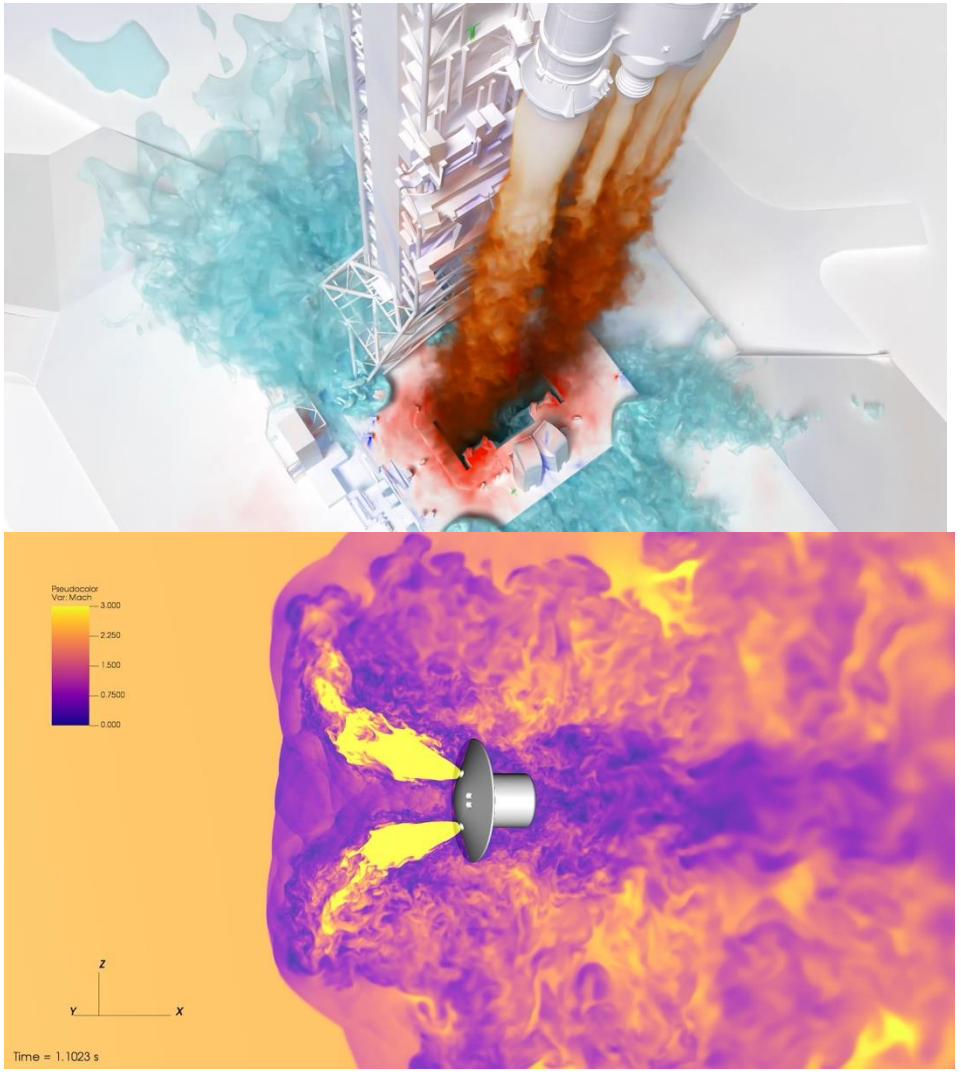
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Motivation

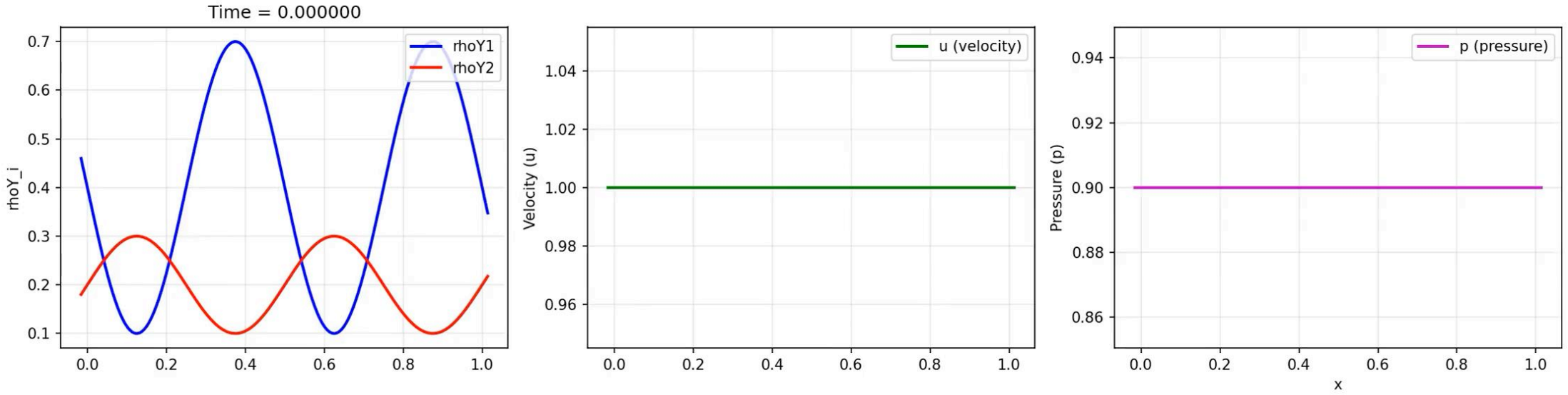
- Multi-species and multi-phase flows are used to model many physical phenomena across a variety of fields.

- 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

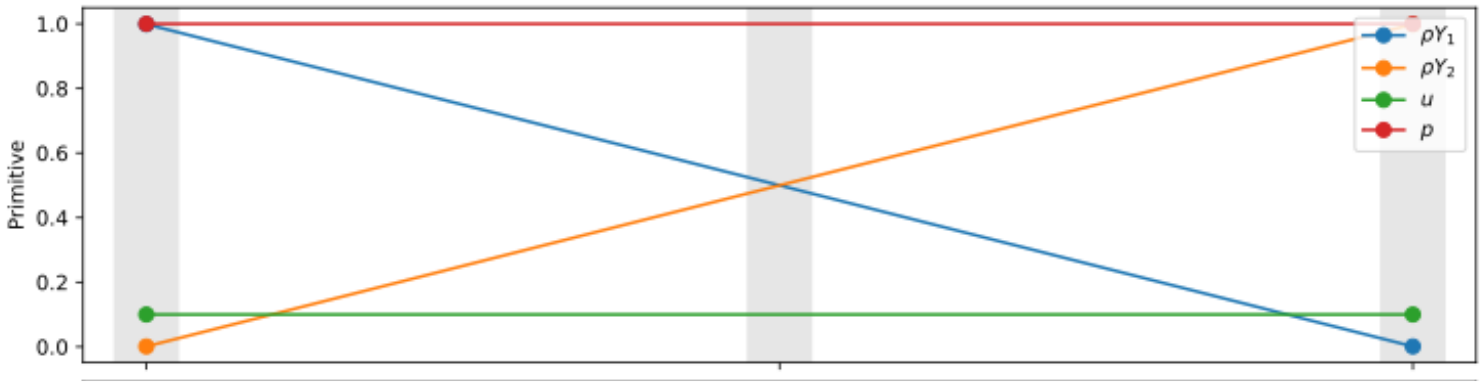
- Long time stability and accuracy of these multi-fluid simulations are compromised by spurious pressure oscillations



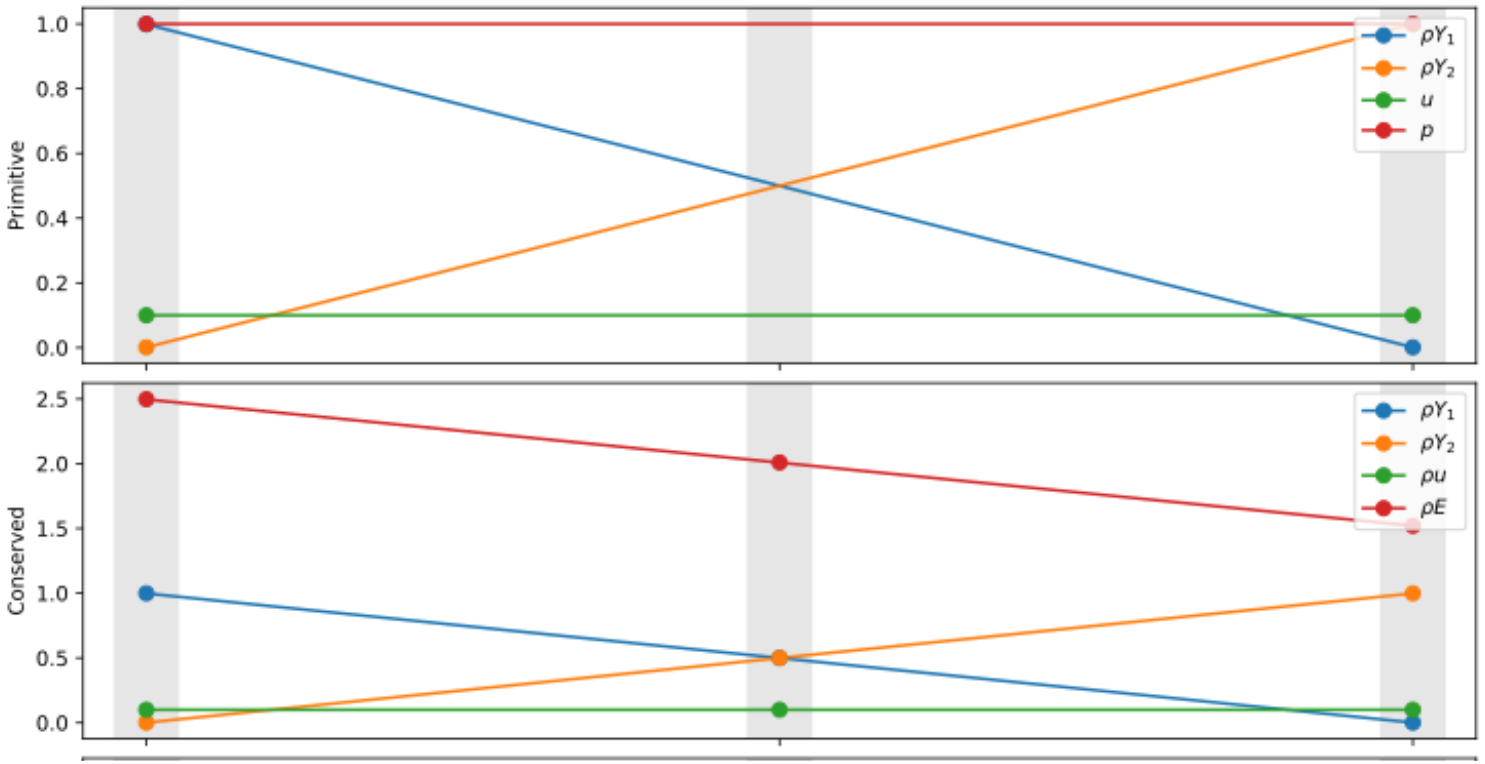
Motivation


Time = 0.000000
rhoY1
rhoY2
rhoY_i
u (velocity)
Velocity (u)
p (pressure)
Pressure (p)
x

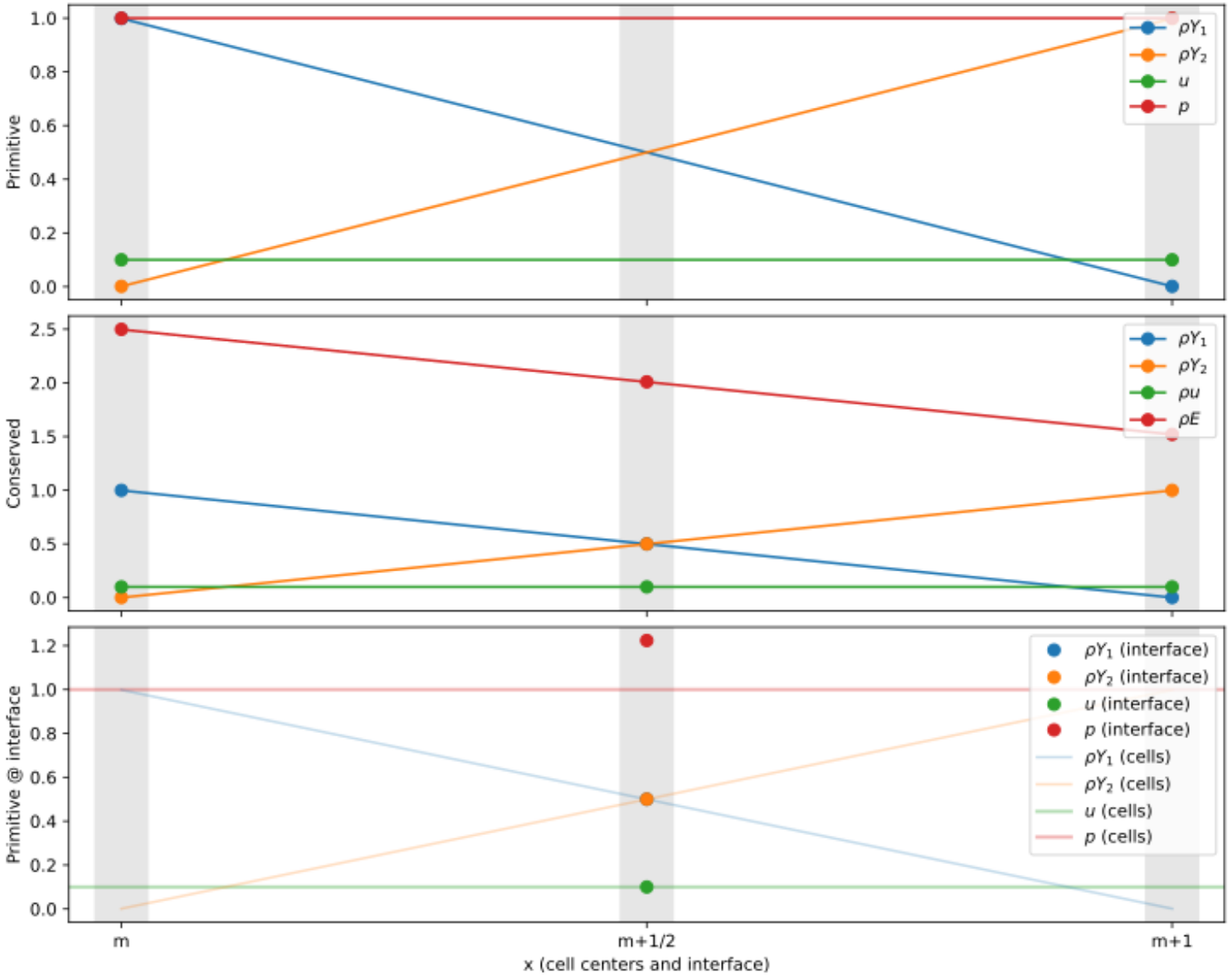
Motivation



Motivation


Primitive
1.0
0.8
0.6
0.4
0.2
0.0
ρY_1
ρY_2
u
p
Conserved
2.5
2.0
1.5
1.0
0.5
0.0
ρY_1
ρY_2
ρu
ρE

Motivation


Primitive
Conserved
Primitive @ interface
x (cell centers and interface)
m
m+1/2
m+1
ρY_1
ρY_2
u
p
ρu
ρE
ρY_1 (interface)
ρY_2 (interface)
u (interface)
p (interface)
ρY_1 (cells)
ρY_2 (cells)
u (cells)
p (cells)

Existing Methods

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 and high-order approximate

Outline

1. **Pressure In-Equilibrium Analysis**
2. Extension of APEC to High-Order
3. Spatially Exact PEP Scheme
4. Results

Two-Fluid 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

- Pressure Equilibrium Property (PEP) is analyzed by assuming the flow starts with uniform velocity and pressure

- By analyzing a timestep, we're interested in the accrual of these errors
  - Any pressure drift is numerical

- Goal

$$u_m^{n+1} - u_m^n = 0,$$
$$p_m^{n+1} - p_m^n = 0.$$

Semi-Discrete Analysis of Pressure Error

- Apply spatial discretization to obtain an ODE system. Note: u = f(ρu, ρ)

$$u_m^{n+1} - u_m^n = \left(\frac{\partial u}{\partial(\rho u)}\right)_\rho^n \left((\rho u)_m^{n+1} - (\rho u)_m^n\right) + \left(\frac{\partial u}{\partial \rho}\right)_{\rho u}^n \left(\rho_m^{n+1} - \rho_m^n\right) + O(\Delta t^2)$$

$$u_m^{n+1} - u_m^n = -\frac{1}{\rho_m^n}\left(F_{\rho u} - U_0 F_\rho\right)_m^n \Delta t + O(\Delta t^2)$$

- Velocity-Equilibrium Condition (automatically satisfied)

$$\rho_{m+\frac{1}{2}} = \sum_i (\rho Y_i)_{m+\frac{1}{2}}$$

Pressure-Equilibrium Condition

- We can analyze pressure in the same way: p = f(ρe, ρY_1, ρY_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 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

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

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

PEP Criterion

To satisfy the PEP 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

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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

- APEC can be applied to any method
- The original formulation is built on the central Kinetic Energy Entropy Preserving (KEEP) scheme:

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

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

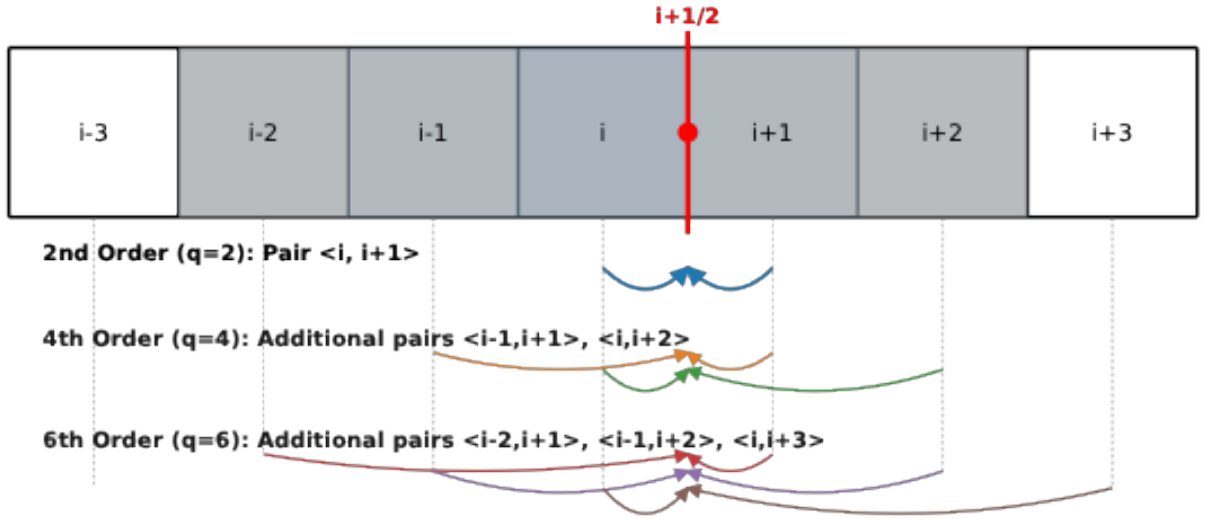
High-Order APEC

High-order convective flux[1]:

$$\widetilde{\mathcal{F}}_{\phi}\Big|_{\left(m\pm\frac{1}{2}\right)} \equiv 2\sum_{i_s=1}^{q/2} a_{q,i_s} \sum_{\ell=0}^{i_s-1} \frac{\rho|_{(m\mp\ell)} + \rho|_{(m\mp\ell\pm i_s)}}{2} \frac{\phi|_{(m\mp\ell)} + \phi|_{(m\mp\ell\pm i_s)}}{2} \frac{u|_{(m\mp\ell)} + u|_{(m\mp\ell\pm i_s)}}{2},$$

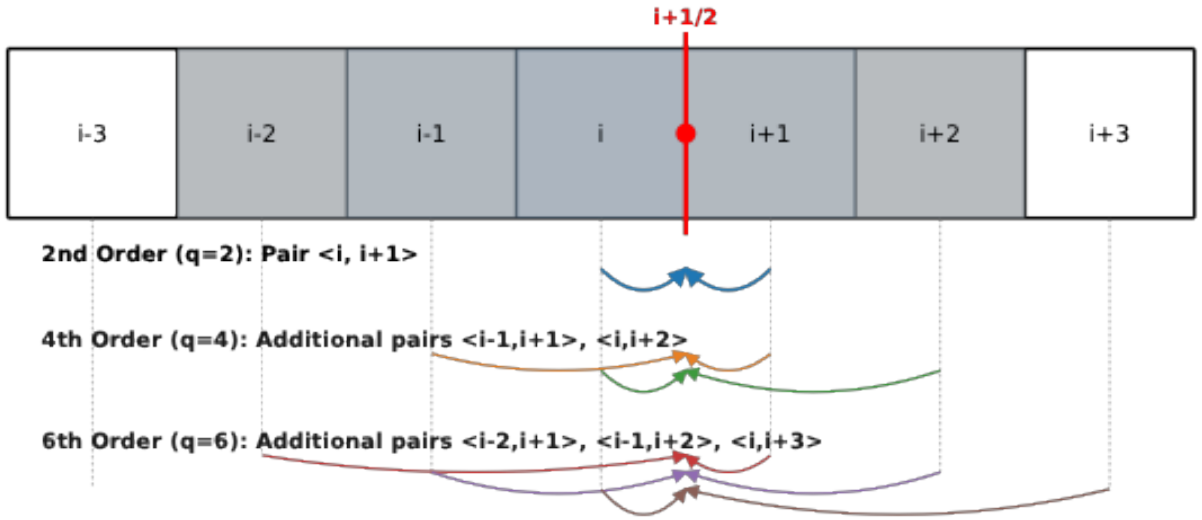
Order	Coefficients			
q	$a_{q,1}$	$a_{q,2}$	$a_{q,3}$	$a_{q,4}$
2	$\frac{1}{2}$			
4	$\frac{2}{3}$	$-\frac{1}{12}$		
6	$\frac{3}{4}$	$-\frac{3}{20}$	$\frac{1}{60}$	
8	$\frac{4}{5}$	$-\frac{1}{5}$	$\frac{4}{105}$	$-\frac{1}{280}$

Extending fluxes to high-order follows the pattern:



[1] *High-order accurate kinetic-energy and entropy preserving (KEEP) schemes on curvilinear grids* (Kuya et al., 2021)

High-Order APEC



Extending the two-point flux of ρe to high-order we can also correct each sub-interface

$$\rho e\big|^{\text{APEC } \mathcal{O}(q)}_{m+\frac{1}{2}} \equiv 2\sum_{i_s=1}^{q/2} a_{q,i_s} \sum_{\ell=0}^{i_s-1} \frac{\rho e\big|_{(m\mp\ell)} + \rho e\big|_{(m\mp\ell\pm i_s)}}{2} - \underbrace{\sum_{i=1}^{N} \left[\frac{\left(\frac{\partial \rho e}{\partial \rho Y_i}\right)_{\rho Y_{j\neq i},p}\Big|_{(m\mp\ell)} - \left(\frac{\partial \rho e}{\partial \rho Y_i}\right)_{\rho Y_{j\neq i},p}\Big|_{(m\mp\ell\pm i_s)}}{2} \frac{\rho Y_i\big|_{(m\mp\ell)} - \rho Y_i\big|_{(m\mp\ell\pm i_s)}}{2} \right]}_{\text{Correction}}.$$

High-Order APEC

- Extends APEC to formally high-order
- Fully conservative
- Minimal small change
- EOS Agnostic

$$C_1|^{\text{APEC }\mathcal{O}(q)}_{m+\frac{1}{2}} = 2\sum_{i_s=1}^{q/2} a_{q,i_s} \sum_{\ell=0}^{i_s-1} \frac{\rho Y_1|_{(m\mp\ell)} + \rho Y_1|_{(m\mp\ell\pm i_s)}}{2} \frac{u|_{(m\mp\ell)} + u|_{(m\mp\ell\pm i_s)}}{2}$$

$$C_2|^{\text{APEC }\mathcal{O}(q)}_{m+\frac{1}{2}} = 2\sum_{i_s=1}^{q/2} a_{q,i_s} \sum_{\ell=0}^{i_s-1} \frac{\rho Y_2|_{(m\mp\ell)} + \rho Y_2|_{(m\mp\ell\pm i_s)}}{2} \frac{u|_{(m\mp\ell)} + u|_{(m\mp\ell\pm i_s)}}{2}$$

$$M|^{\text{APEC }\mathcal{O}(q)}_{m+\frac{1}{2}} = 2\left(\rho|^{\text{APEC }\mathcal{O}(q)}_{m+\frac{1}{2}}\right) \sum_{i_s=1}^{q/2} a_{q,i_s} \sum_{\ell=0}^{i_s-1} \left[\frac{u|_{(m\mp\ell)} + u|_{(m\mp\ell\pm i_s)}}{2}\right]^2$$

$$\Pi|^{\text{APEC }\mathcal{O}(q)}_{m+\frac{1}{2}} = 2\sum_{i_s=1}^{q/2} a_{q,i_s} \sum_{\ell=0}^{i_s-1} \frac{p|_{(m\mp\ell)} + p|_{(m\mp\ell\pm i_s)}}{2}$$

$$K|^{\text{APEC }\mathcal{O}(q)}_{m+\frac{1}{2}} = 2\left(\rho|^{\text{APEC }\mathcal{O}(q)}_{m+\frac{1}{2}}\right) \sum_{i_s=1}^{q/2} a_{q,i_s} \sum_{\ell=0}^{i_s-1} \frac{u|_{(m\mp\ell)} + u|_{(m\mp\ell\pm i_s)}}{2} \frac{u|_{(m\mp\ell)}\ u|_{(m\mp\ell\pm i_s)}}{2}$$

$$I|^{\text{APEC }\mathcal{O}(q)}_{m+\frac{1}{2}} = 2\left(\rho e|^{\text{APEC }\mathcal{O}(q)}_{m+\frac{1}{2}}\right) \sum_{i_s=1}^{q/2} a_{q,i_s} \sum_{\ell=0}^{i_s-1} \frac{u|_{(m\mp\ell)} + u|_{(m\mp\ell\pm i_s)}}{2}$$

$$S|^{\text{APEC }\mathcal{O}(q)}_{m+\frac{1}{2}} = 2\sum_{i_s=1}^{q/2} a_{q,i_s} \sum_{\ell=0}^{i_s-1} \frac{u|_{(m\mp\ell)}\ p|_{(m\mp\ell\pm i_s)} + u|_{(m\mp\ell\pm i_s)}\ p|_{(m\mp\ell)}}{2}$$

Taylor Expansion of APEC

In the paper we Taylor expand the flux of pressure error

With APEC, we see smaller coefficients for orders 2,4,6,8

$$f_{PE}^{\text{KEEP } \mathcal{O}(2)} = \sum_{i=1}^{N} \left[\frac{1}{3} \frac{\partial}{\partial x} \left(\frac{\partial \rho e}{\partial \rho Y_i} \right) \frac{\partial^2 (\rho Y_i)}{\partial x^2} + \frac{1}{6} \frac{\partial^2}{\partial x^2} \left(\frac{\partial \rho e}{\partial \rho Y_i} \right) \frac{\partial (\rho Y_i)}{\partial x} \right],$$

$$f_{PE}^{\text{APEC } \mathcal{O}(2)} = \sum_{i=1}^{N} \left[\frac{1}{12} \frac{\partial}{\partial x} \left(\frac{\partial \rho e}{\partial \rho Y_i} \right) \frac{\partial^2 (\rho Y_i)}{\partial x^2} - \frac{1}{12} \frac{\partial^2}{\partial x^2} \left(\frac{\partial \rho e}{\partial \rho Y_i} \right) \frac{\partial (\rho Y_i)}{\partial x} \right].$$

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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

- The raw condition number of A is scale dependent and misleading for non-normalized systems

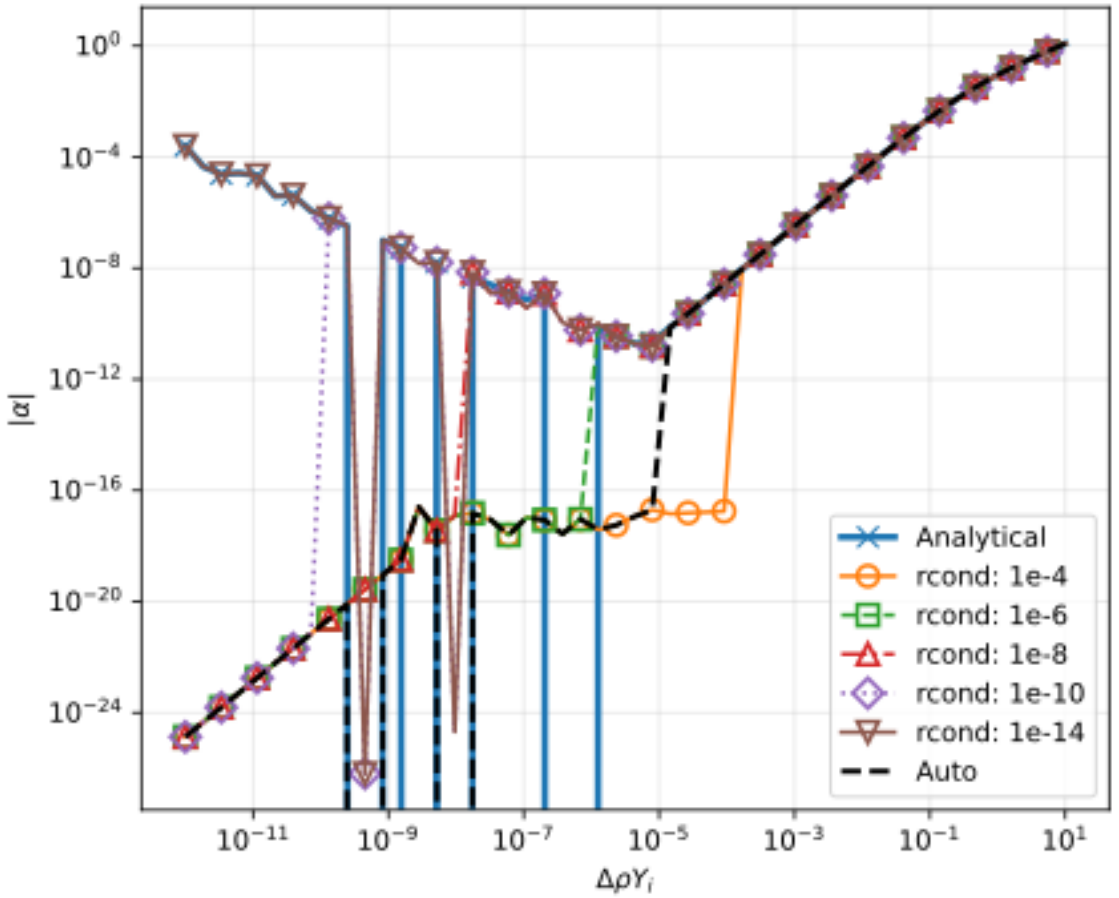
$$\widetilde{A}_{m+\frac{1}{2}} = \begin{bmatrix} \dfrac{\epsilon_1^{m+1} - \epsilon_2^{m+1}}{\sqrt{\max\left(|\epsilon_1^m - \epsilon_2^m|, |\epsilon_1^{m+1} - \epsilon_2^{m+1}|, 1\right)}} & -1 \\ -\dfrac{\epsilon_1^m - \epsilon_2^m}{\sqrt{\max\left(|\epsilon_1^m - \epsilon_2^m|, |\epsilon_1^{m+1}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

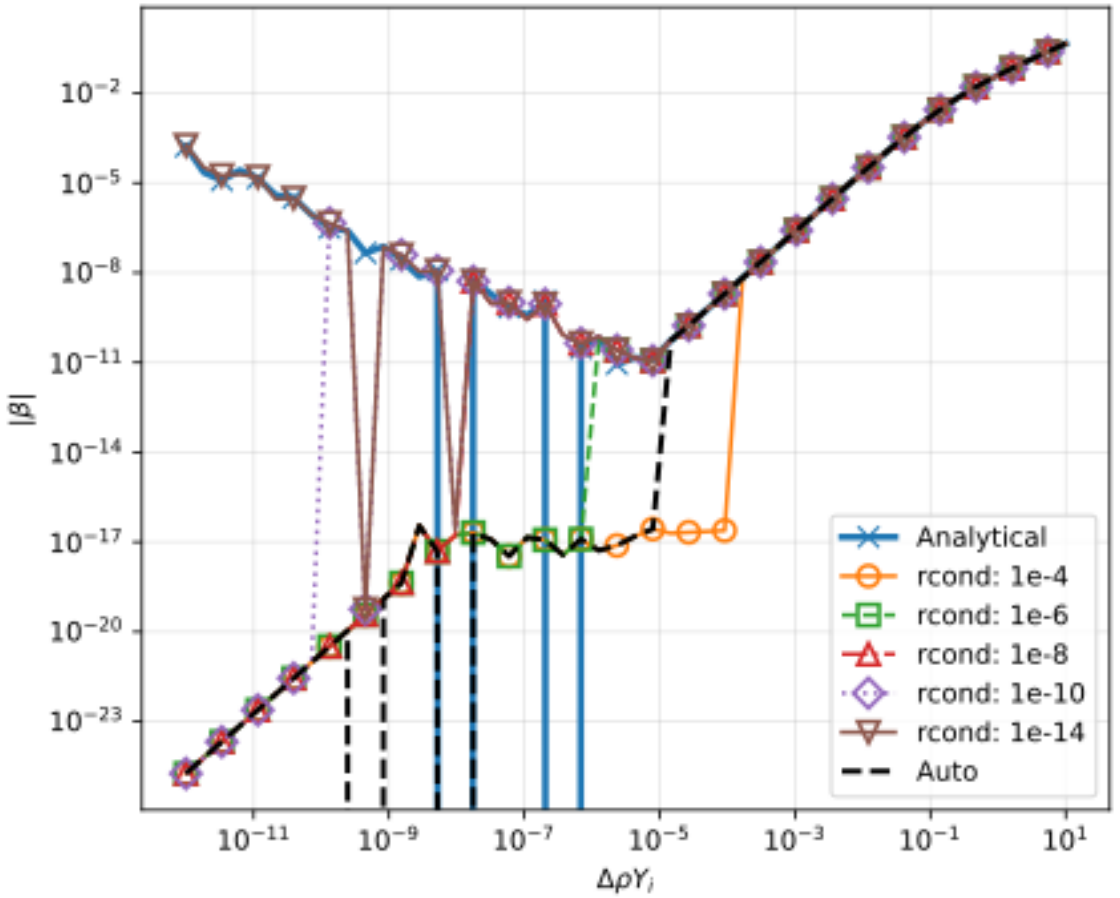
- We solve for eigenvalues of G as a scale independent measure of condition number:

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

- 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





Outline

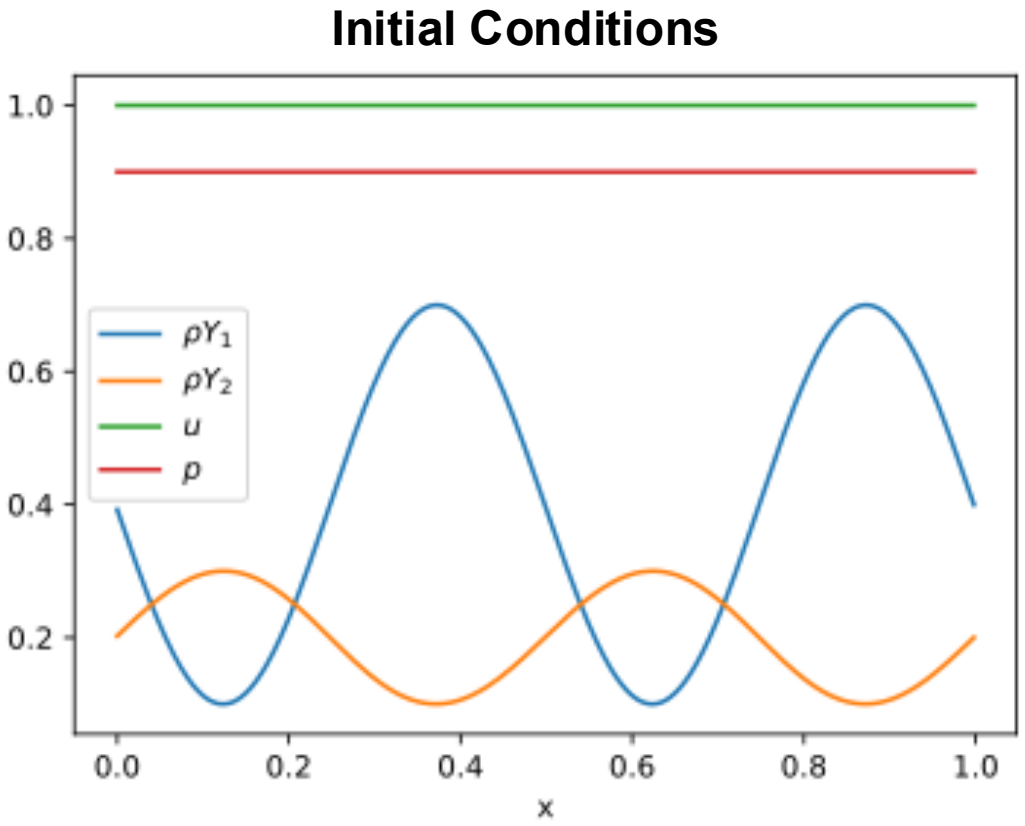
1. Pressure In-Equilibrium Analysis
2. Extension of APEC to High-Order
3. Spatially Exact PEP Scheme
4. **Results**

Ideal Gas Test Case

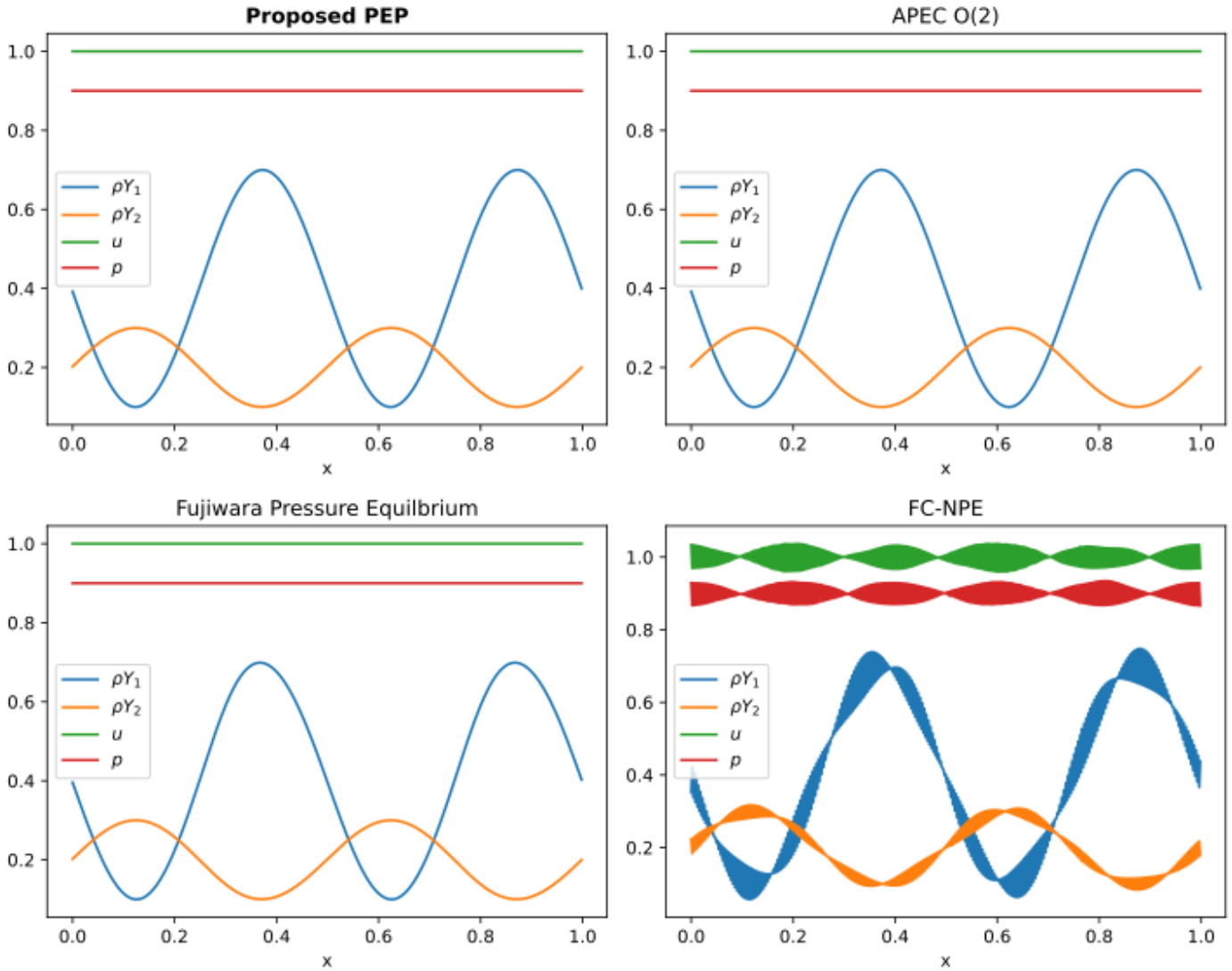
Fluid 1: γ = 1.4, Molecular Weight = 28 g/mol
Fluid 2: γ = 1.66, Molecular Weight = 4 g/mol

501 cells
4th Order Runge-Kutta
CFL = 0.6
Periodic BCs

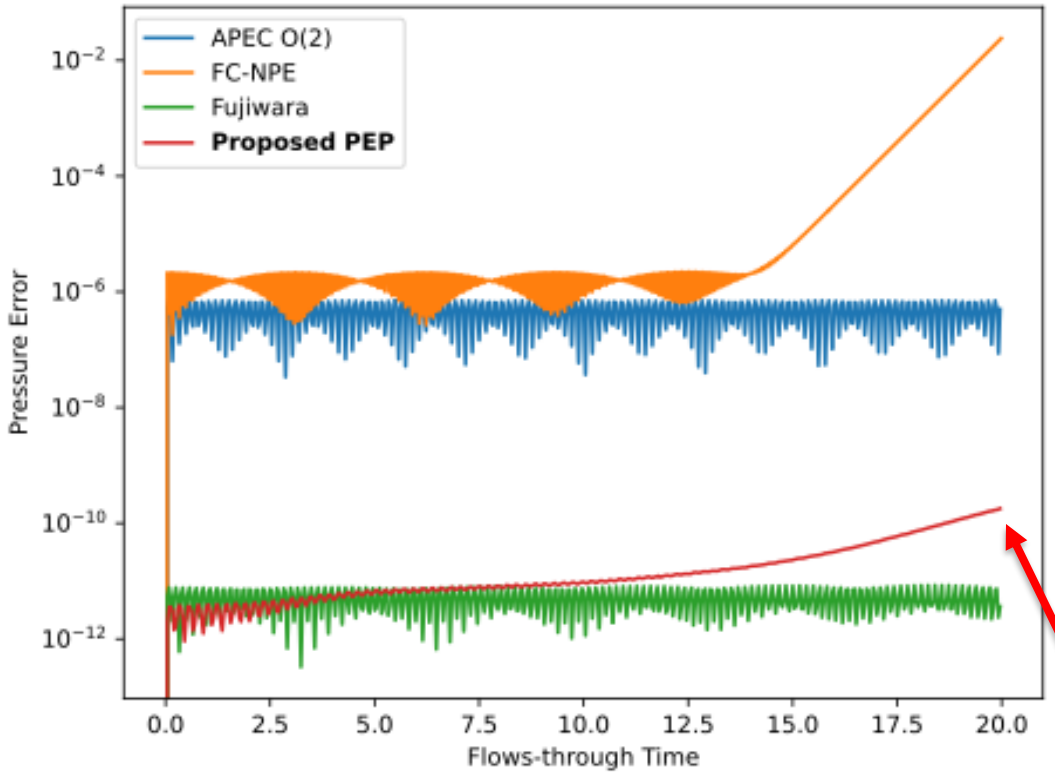
Equation of State: $\rho e = \frac{P}{\bar{\gamma} - 1}$

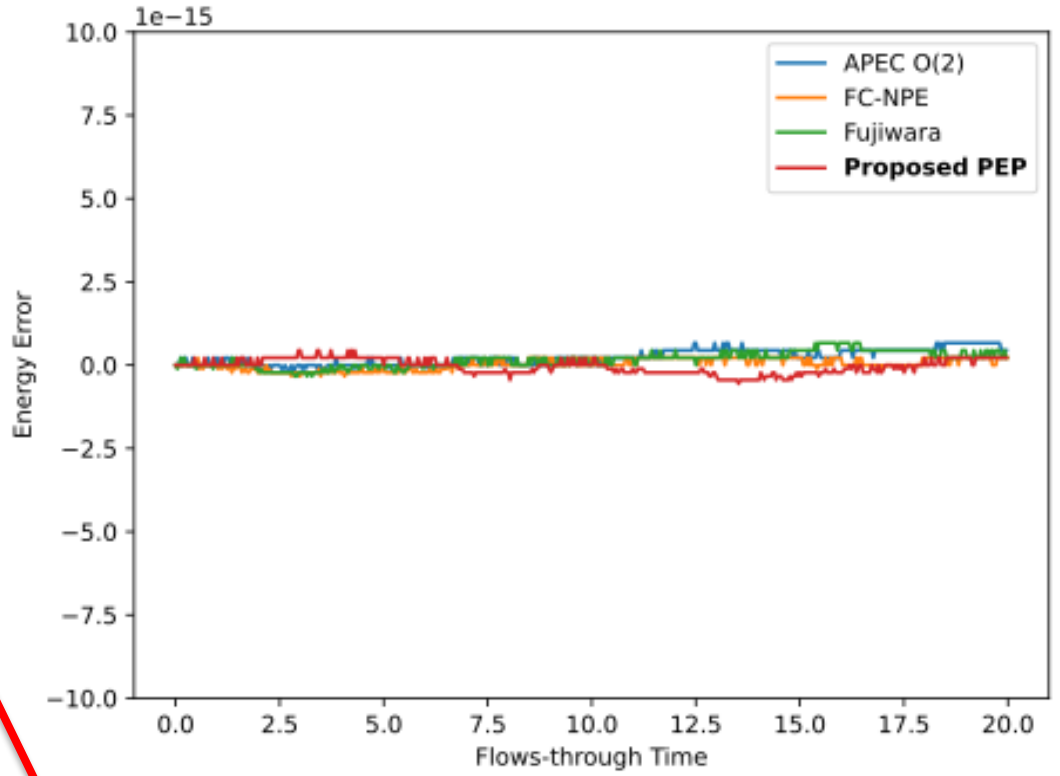


Ideal Gas Test Case at 20 CTUs



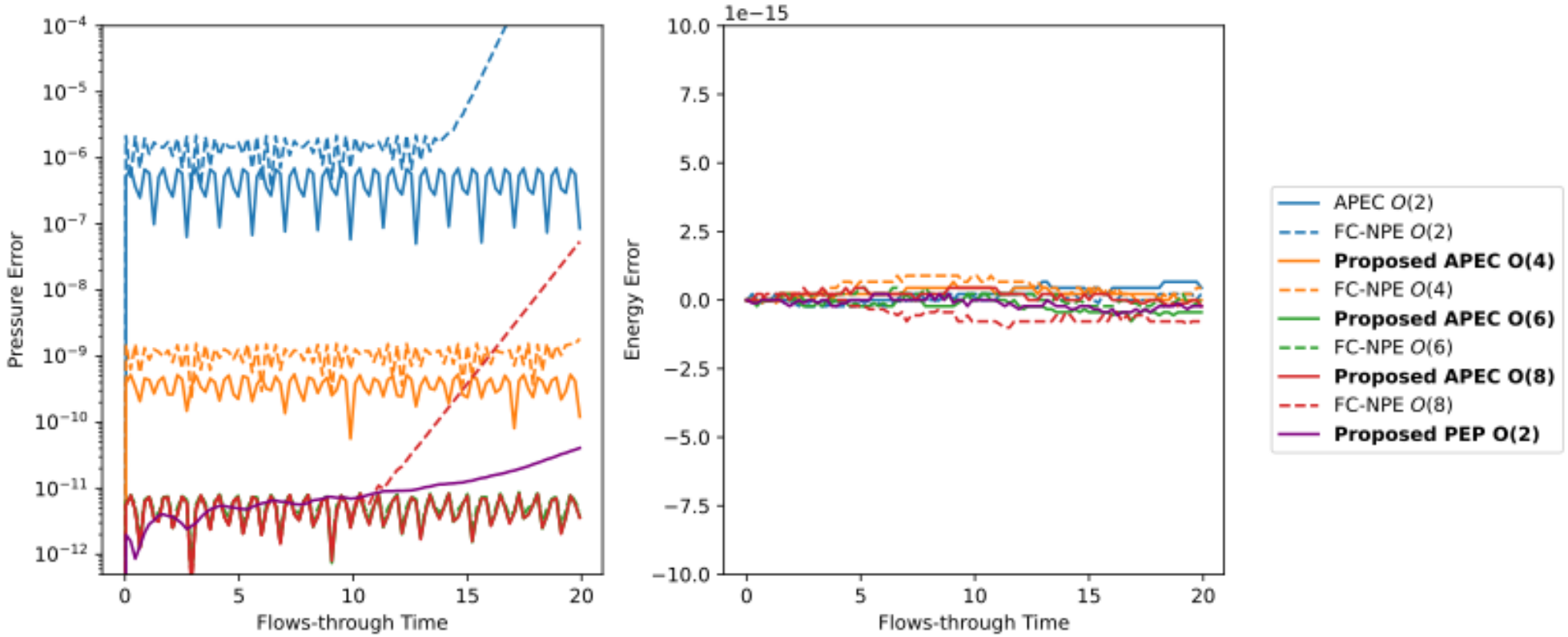
Ideal Gas Test Case at 20 CTUs





Increase in pressure error due to pseudo-inverse

Ideal Gas Test Case at 20 CTUs, High-Order Methods



Stiffened Gas Test Case

Fluid 1: γ = 3.0, Molecular Weight = 18 g/mol

p_∞ = 0.1, q = -0.1

Fluid 2: γ = 1.4, Molecular Weight = 29 g/mol

p_∞ = 0.0, q = 0.0

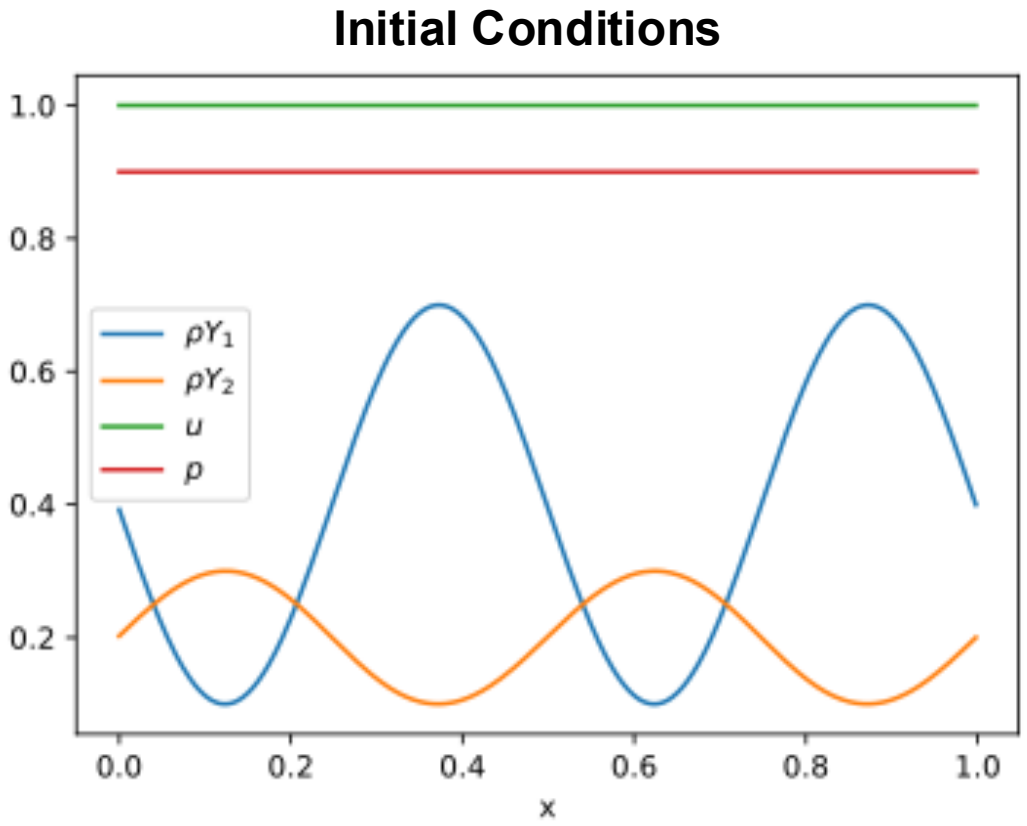
501 cells

4th Order Runge-Kutta

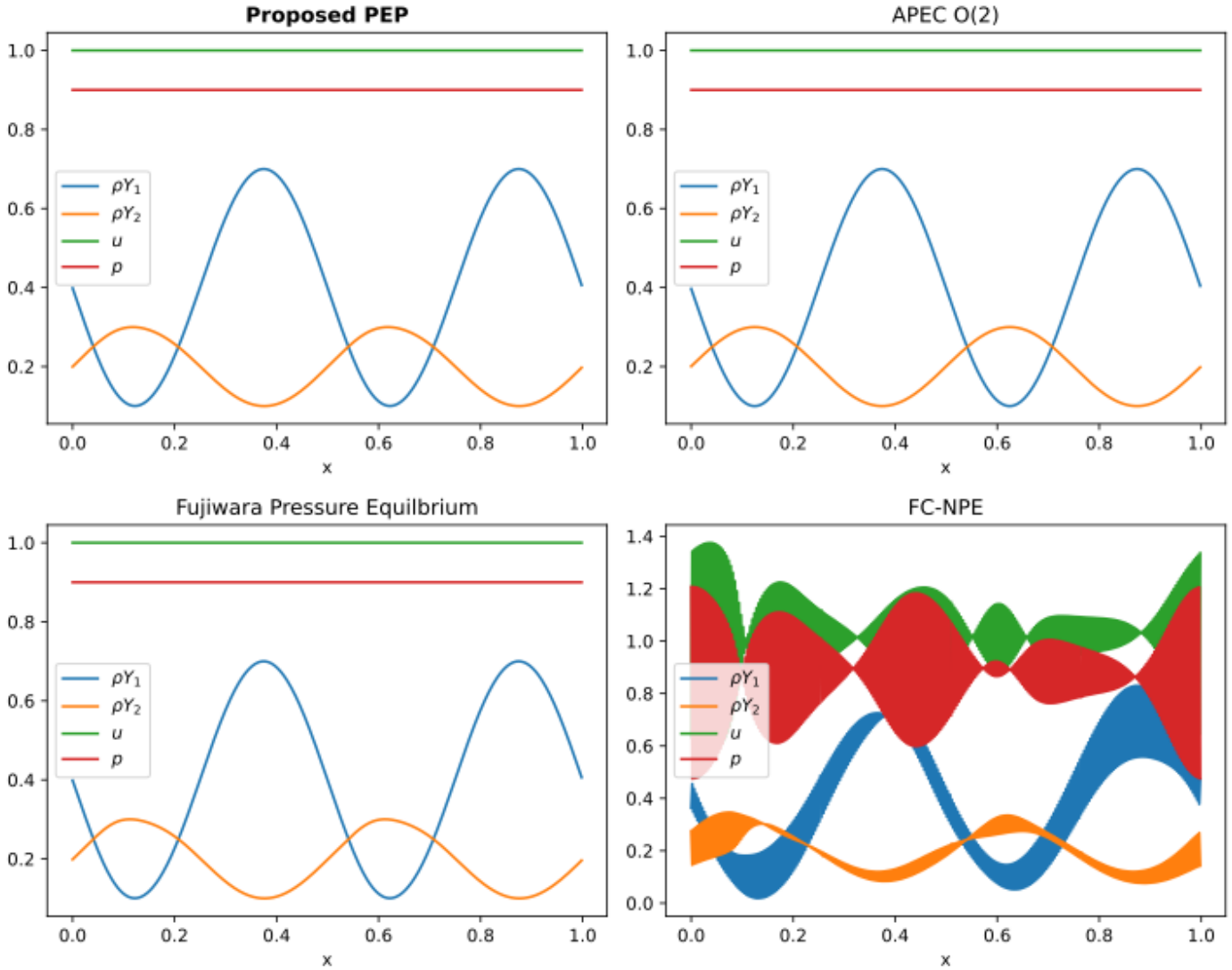
CFL = 0.6

Periodic BCs

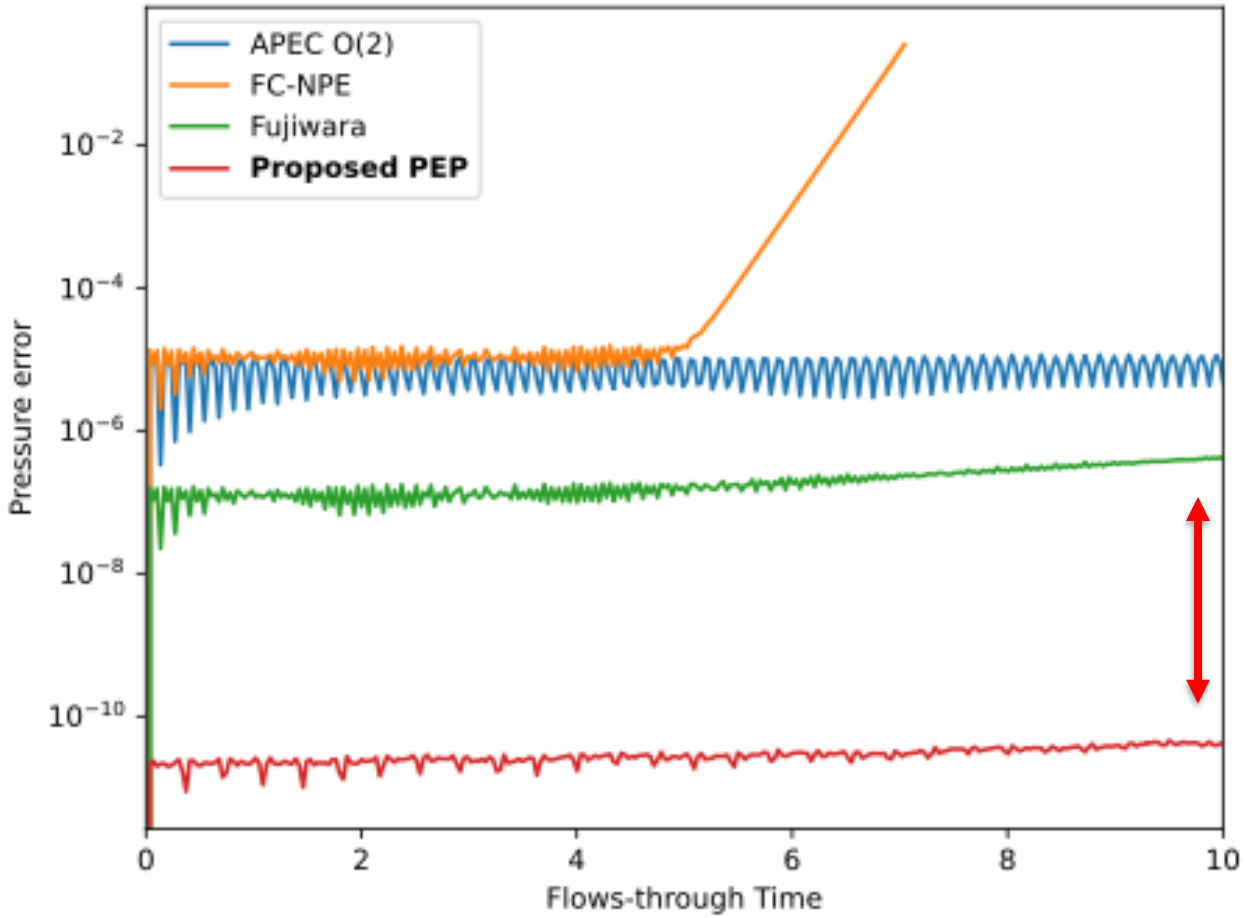
Equation of State: $$\rho e = \frac{p}{\bar{\gamma} - 1} + \bar{A} + \rho \bar{Q},$$



Stiffened Gas Test Case at 7 CTUs

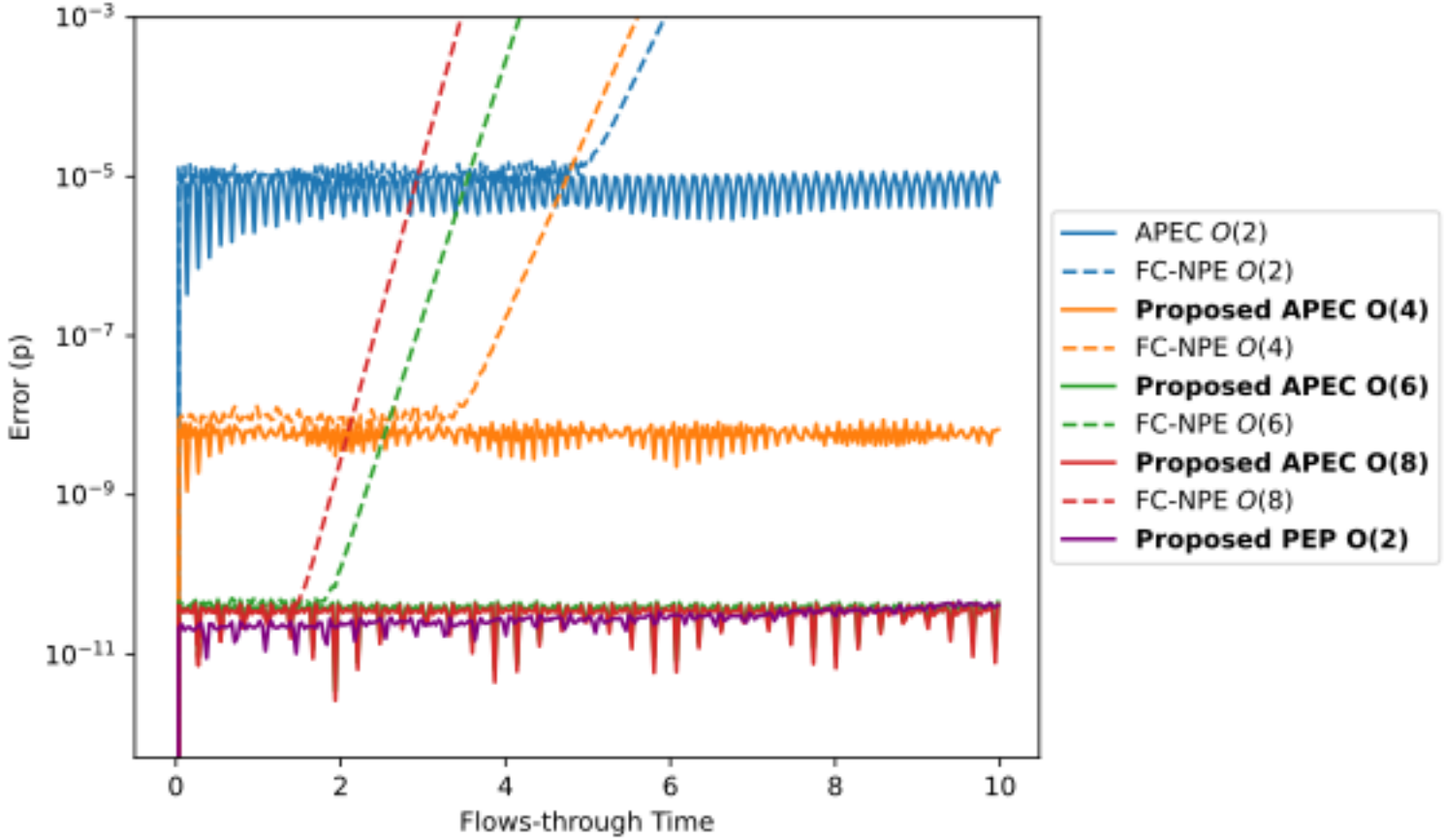


Stiffened Gas Test Case at 7 CTUs



Fujiwara is no longer exact when q is not 0. It is still more accurate than KEEP and APEC

Stiffened Gas Test Case at 7 CTUs



Second order Proposed PEP scheme achieves similar accuracy to 8^{th} order method

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

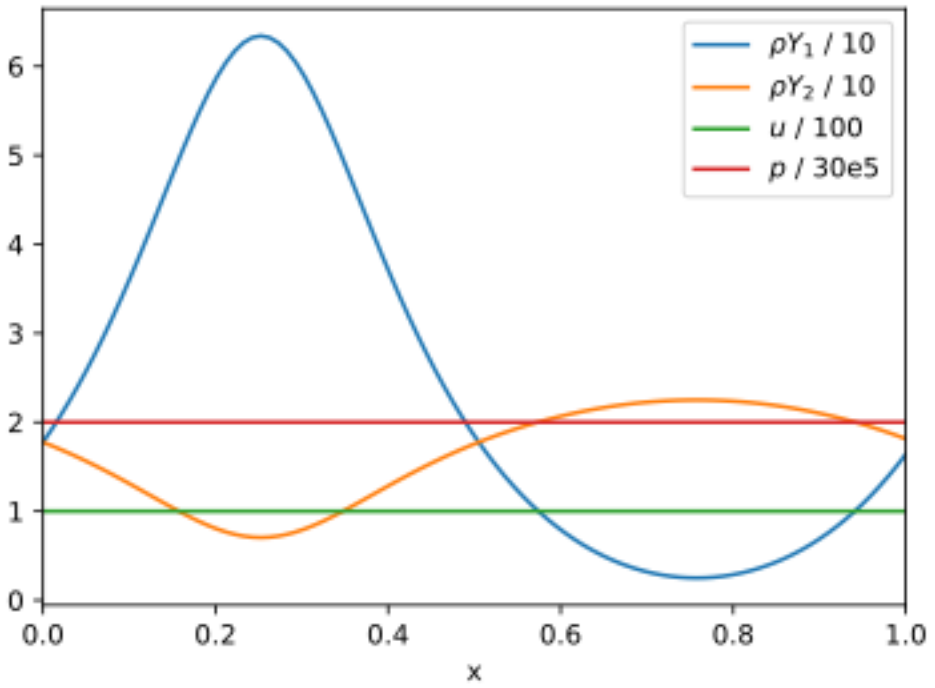
CFL = 0.6

Periodic BCs

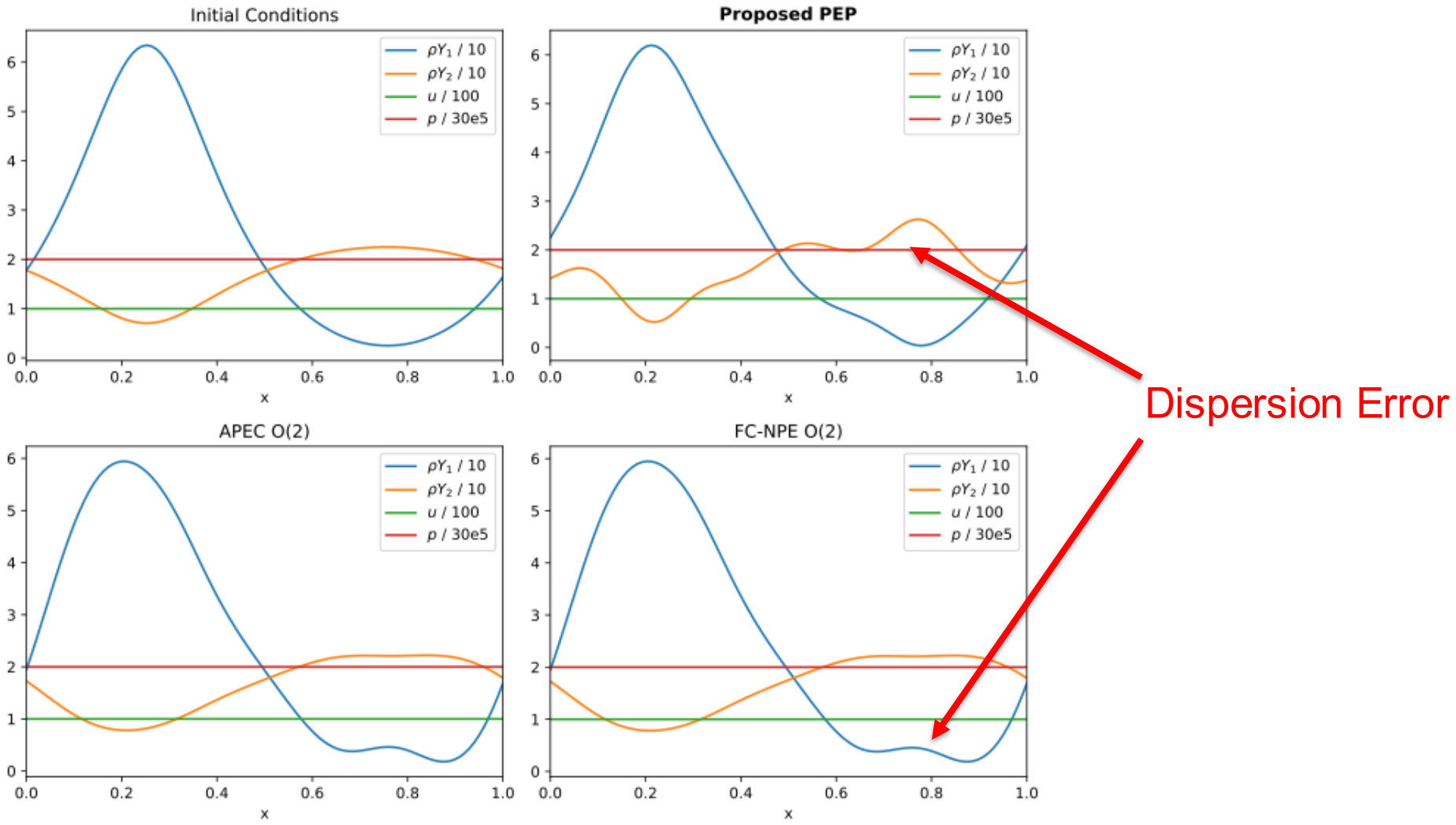
Equation of State: $\left(p + \frac{\bar{a}}{v^2}\right)\left(v - \bar{b}\right) = RT$

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

Initial Conditions

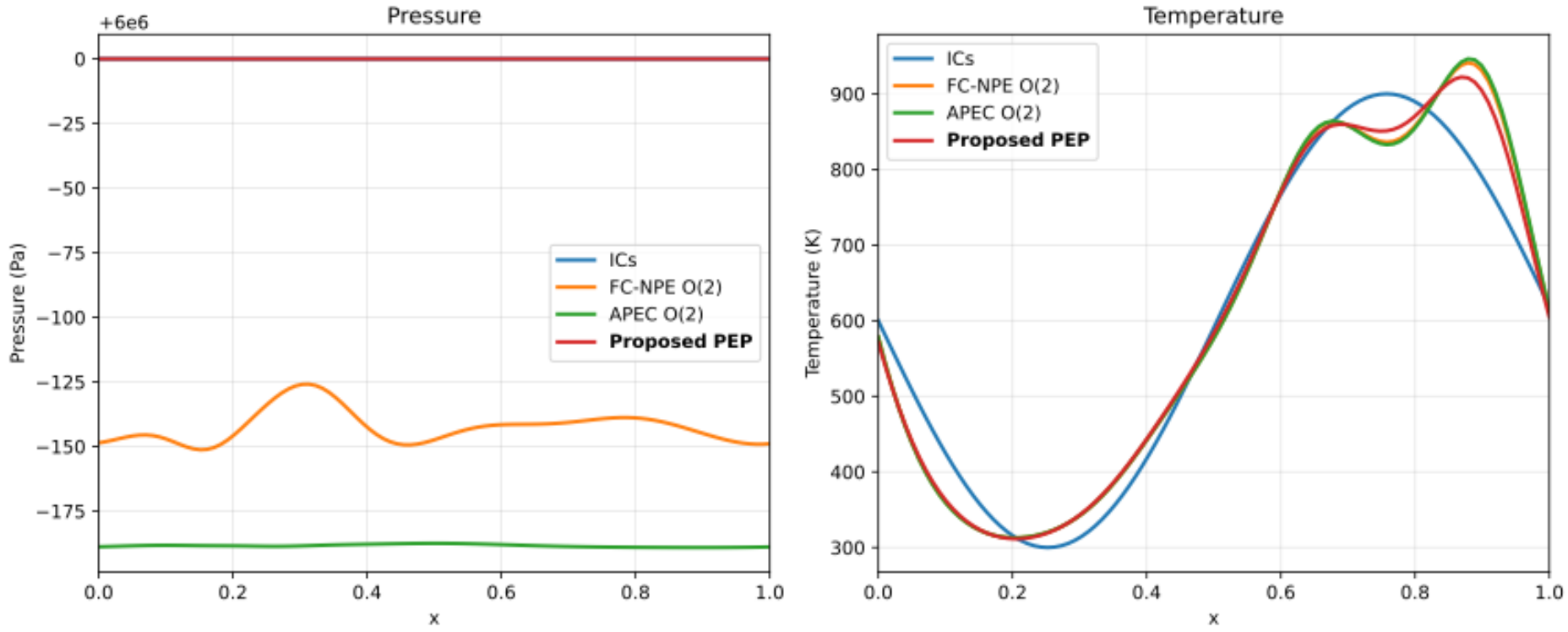


Van der Waals Test Case at 20 CTUs

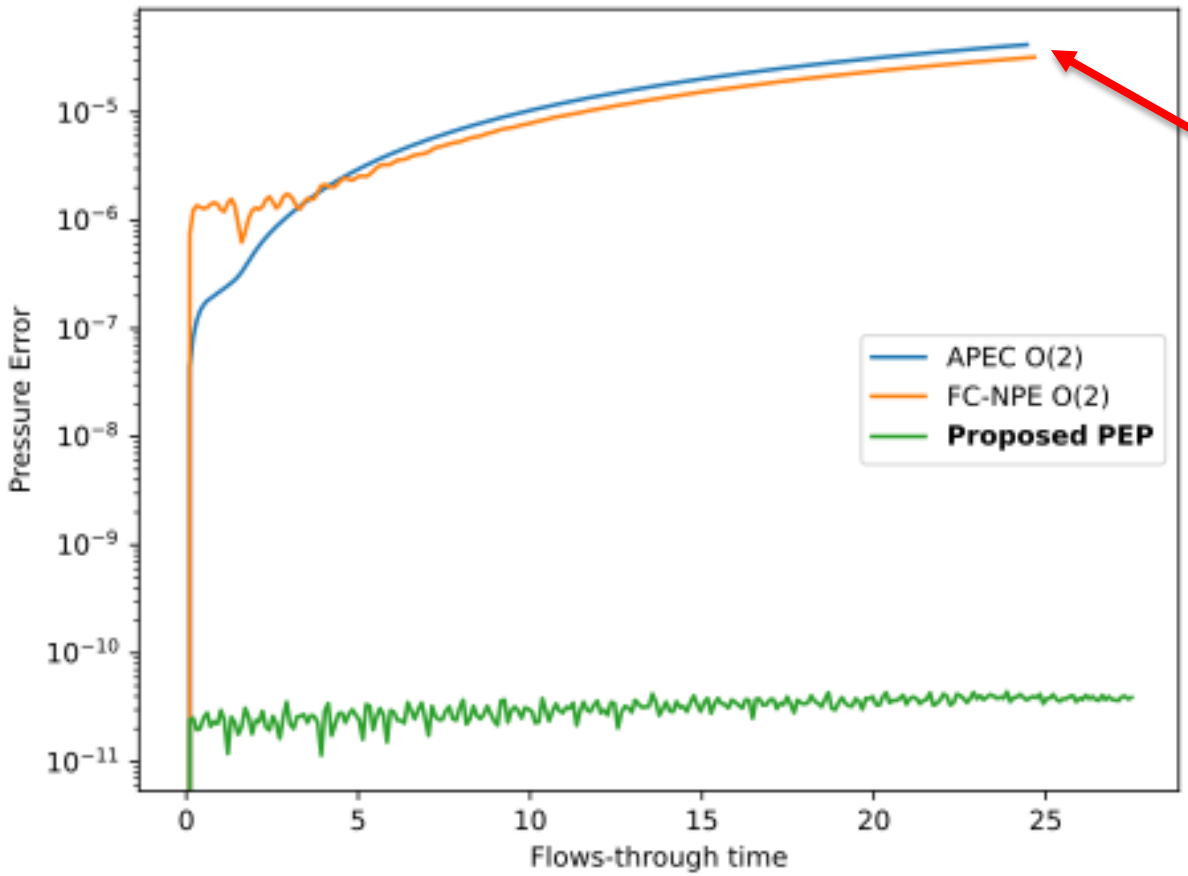


Van der Waals Test Case at 20 CTUs

- Proposed PEP scheme has lowest temperature error. APEC makes corrections by dumping error into temperature. Proposed PEP spreads across temperature and mass fractions
- APEC also has a greater pressure error, but smoother



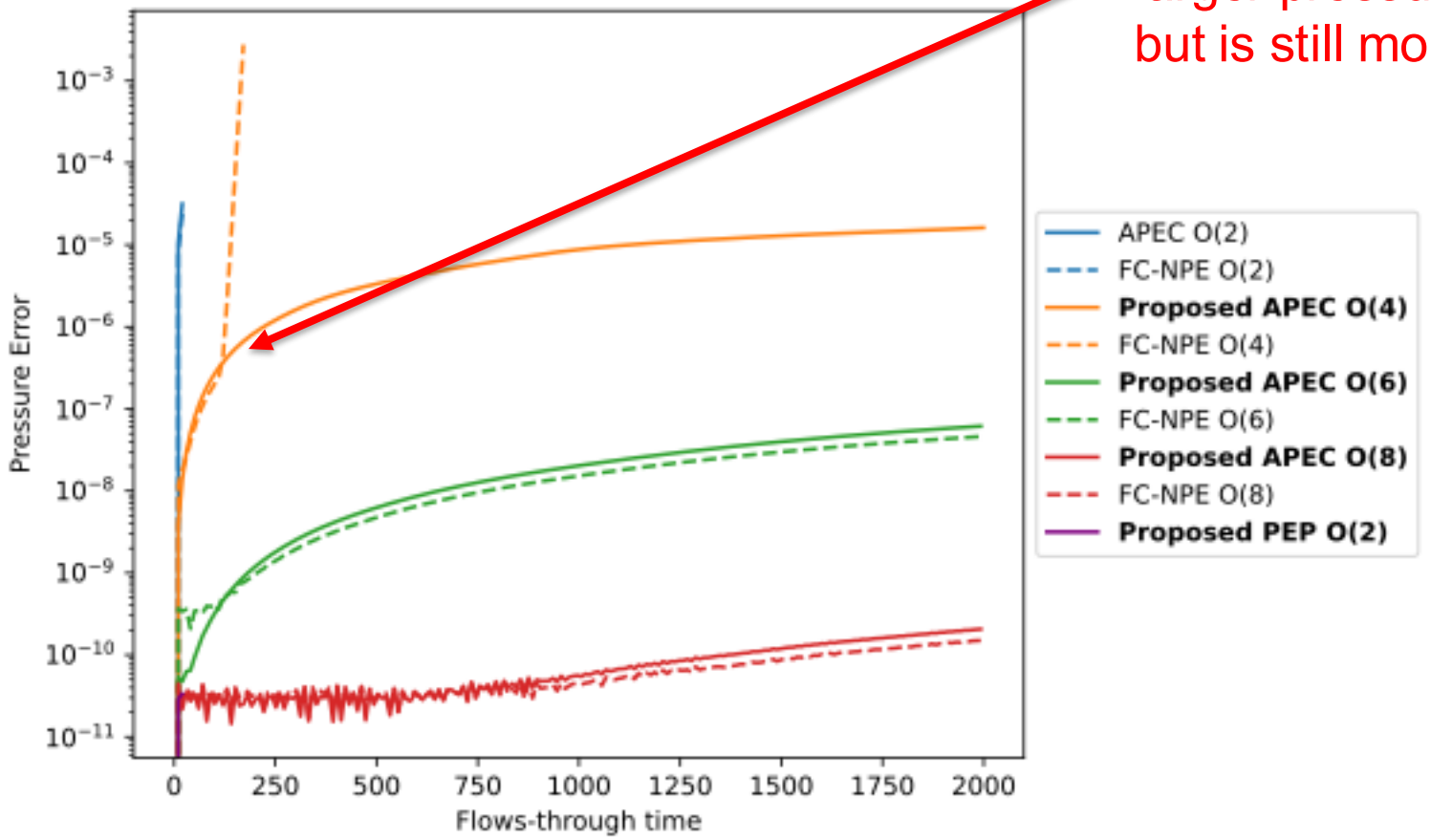
Van der Waals O(2) Fails with Dispersion Error rather than Pressure Error



APEC has slightly larger pressure error

Van der Waals Test Case, High-Order Schemes

APEC has slightly larger pressure error, but is still more stable



Conclusion

We introduce two methods:

1. High-Order extension of APEC Scheme
2. A spatially exact Pressure-Equilbrium-Preserving Scheme

Both methods are:

- 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 for the 3 inviscid advection problems

Future Work

Both methods can be trivially extended to multiple dimensions and multiple species for an arbitrary equation of state

Apply proposed PEP framework to numerical fluxes with shock capturing and diffusion (Riemann solver and hybrid central-upwind schemes)

- This will also help with the failure due to dispersion since it's no longer fully central

We hope to apply these methods in multi-fluid simulations such that there is now no longer a need to sacrifice energy conservation for pressure equilibrium

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)

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Questions