High-Order Data Reconstruction In 1D Hydrodynamics

B08202055 許皓揚
B09202003 陳雙雙

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1D Hydro Code and the Test Problem

The 1 dimensional Hydro code

- MUSCL-Hancock scheme
- HLLC Riemann solver
- Test problem: Sod shock tube, acoustic wave
- Compare results with the analytical solution at end time T=0.1

Initial condition

Left state **Right state**

$$\begin{bmatrix} \rho_L \\ v_L \\ P_L \end{bmatrix} = \begin{bmatrix} 1.0 \\ 0.0 \\ 1.0 \end{bmatrix}, \begin{bmatrix} \rho_R \\ v_R \\ P_R \end{bmatrix} = \begin{bmatrix} 0.125 \\ 0.0 \\ 0.1 \end{bmatrix}$$

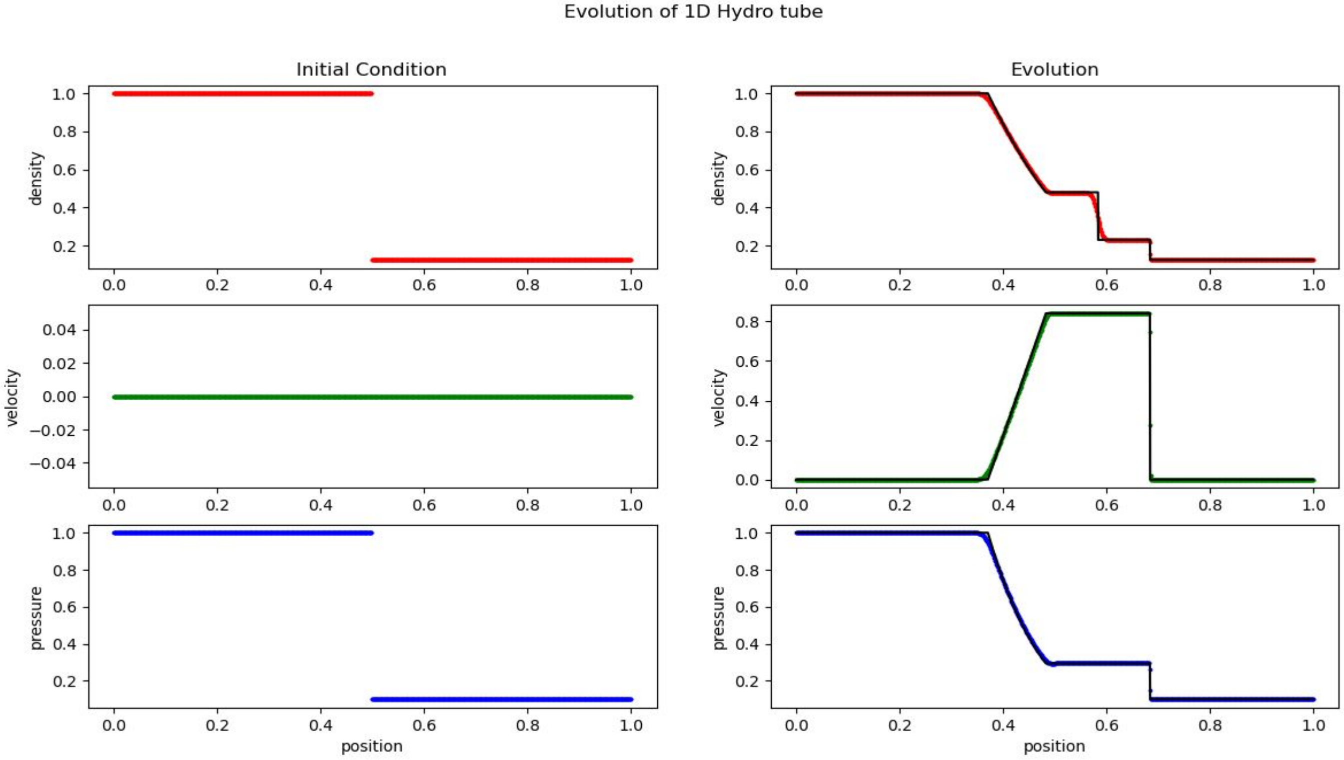
Data Reconstruction Method

- Piecewise constant method (PCM): the original Godunov method
  - First order accurate
- Piecewise linear method (PLM):
  - with van Leer slope limiter to avoid new local extrema
  - should be second order accurate
- Piecewise parabolic method (PPM)
  - should be third order accurate
- Gaussian Process (GP)

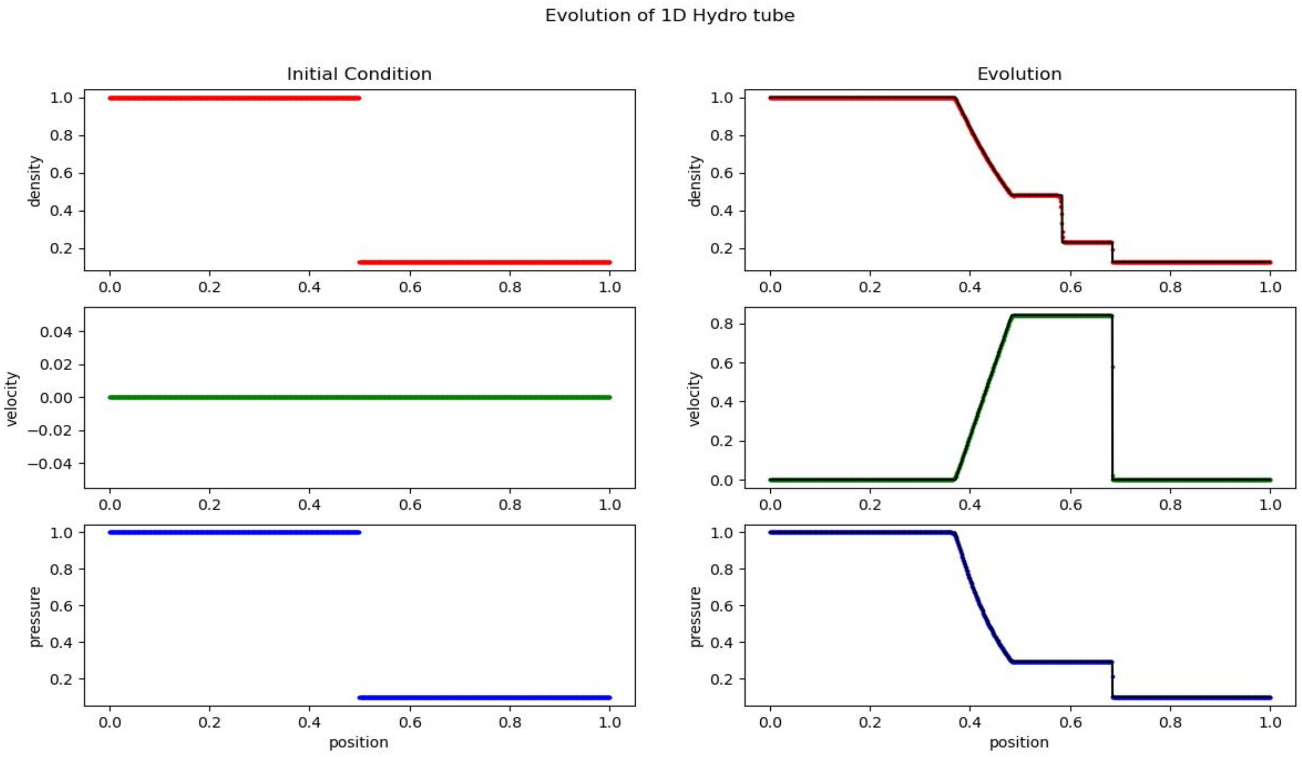
Parallel computation

- Use OpenMP `#   pragma omp parallel for`
- Parallelize the part for calculating Riemann flux, and other minor functions (e.g., computation of sound speed, limited slope, etc).
- For large N (e.g., 1000 or 2000), using 2 threads can cut the wall-clock time in half. However, using 4 threads isn’t faster.
  (Note: Depends on how many CPU cores are in the computer)

Piecewise constant method (PCM) result



Piecewise linear method (PLM) result



Piecewise Parabolic Method (PPM)

Implementation

- Convert conserved variables to primitive variables. Calculate the slope of each cell $\delta \mathbf{w}_i^m$ with van Leer limiter, as in the PLM method.
- Use parabolic interpolation to compute values at the left- and right-side of each cell cell:

$$\mathbf{w}_{L,i} = (\mathbf{w}_i + \mathbf{w}_{i-1})/2 - (\delta \mathbf{w}_i^m + \delta \mathbf{w}_{i-1}^m)/6$$
$$\mathbf{w}_{R,i} = (\mathbf{w}_{i+1} + \mathbf{w}_i)/2 - (\delta \mathbf{w}_{i+1}^m + \delta \mathbf{w}_i^m)/6$$

Implementation

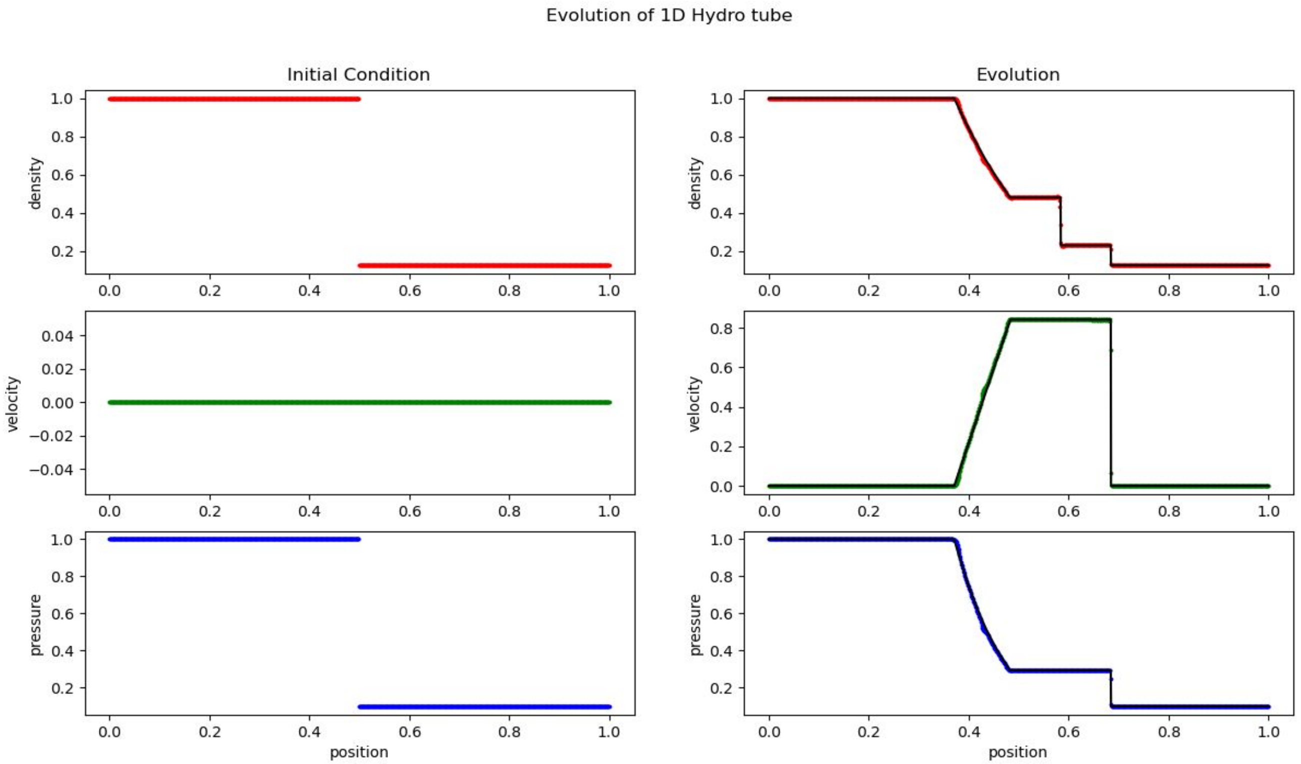
- Monotonicity constraints: Ensure the values on the left- and right-side of cell center lie between neighboring cell-centered values.

$$\text{if } (\mathbf{w}_{R,i}-\mathbf{w}_i)(\mathbf{w}_i-\mathbf{w}_{L,i}) \leq 0: \quad \mathbf{w}_{L,i}=\mathbf{w}_i \ , \ \mathbf{w}_{R,i}=\mathbf{w}_i$$

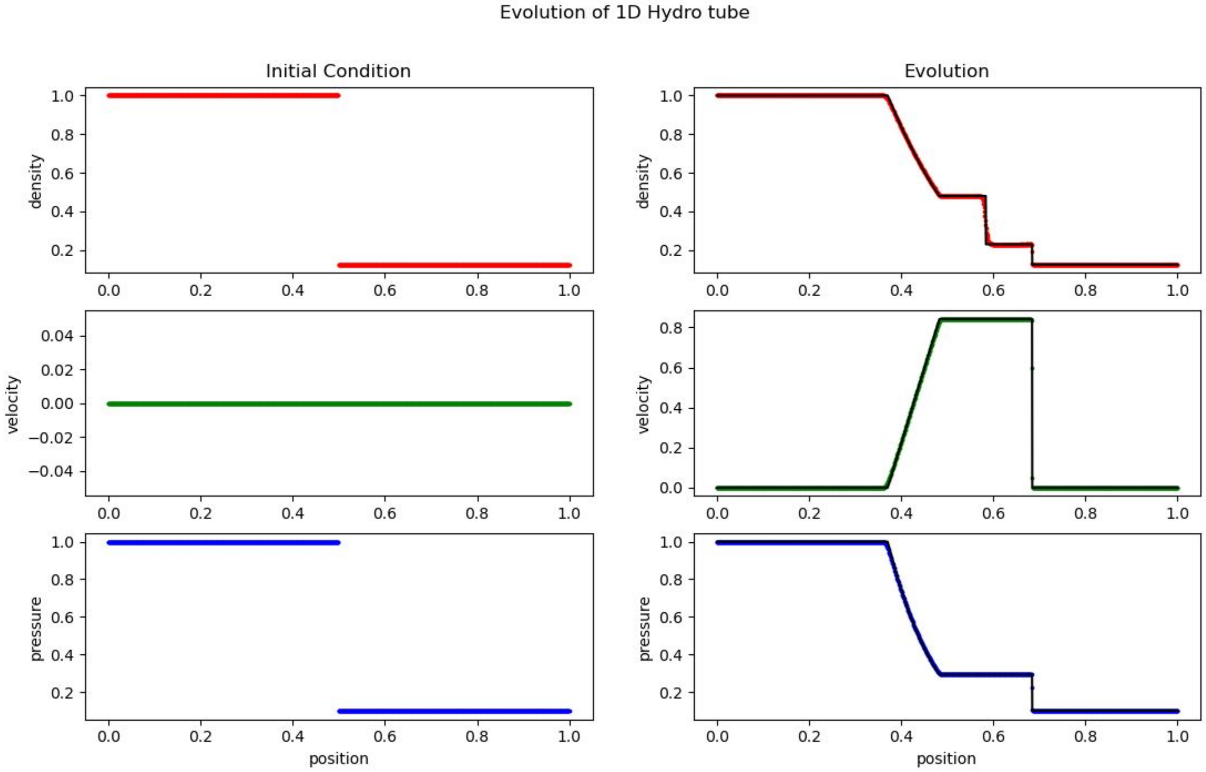
$$\text{if } 6(\mathbf{w}_{R,i}-\mathbf{w}_{L,i})(\mathbf{w}_i-(\mathbf{w}_{L,i}+\mathbf{w}_{R,i})/2) > (\mathbf{w}_{R,i}-\mathbf{w}_{L,i})^2: \ \mathbf{w}_{L,i}=3\mathbf{w}_i-2\mathbf{w}_{R,i}$$

$$\text{if } 6(\mathbf{w}_{R,i}-\mathbf{w}_{L,i})(\mathbf{w}_i-(\mathbf{w}_{L,i}+\mathbf{w}_{R,i})/2) < -(\mathbf{w}_{R,i}-\mathbf{w}_{L,i})^2: \ \mathbf{w}_{R,i}=3\mathbf{w}_i-2\mathbf{w}_{L,i}$$

Piecewise parabolic method (PPM) result



NEW: Piecewise parabolic method (PPM) result



Fix the bug that cause errors at the rarefaction wave.

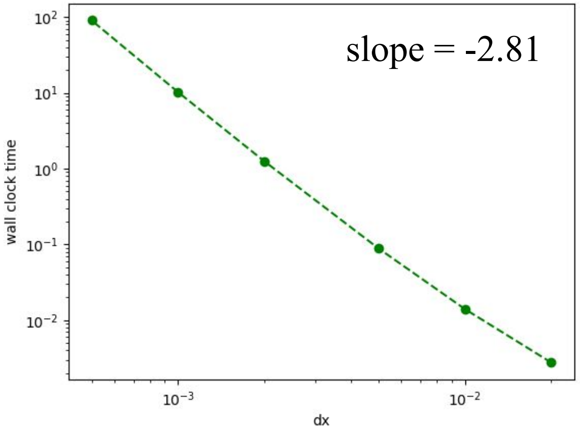
Performance: wall-clock time

threads	PCM	PLM	PPM
1	119.303281	115.460185	115.977558
2	66.330743	64.517736	64.743422
4	57.220275	56.637502	56.538886

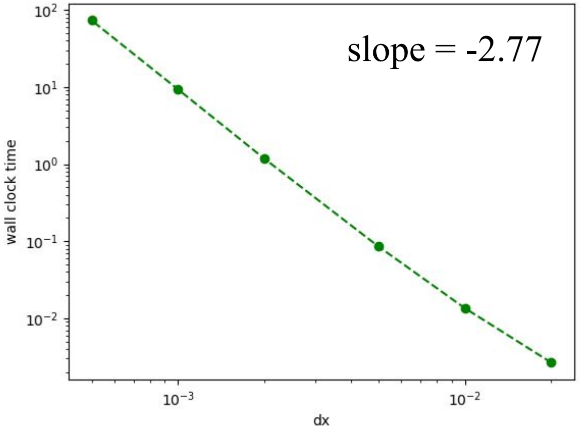
Unit: second

with the number of cells N = 2000

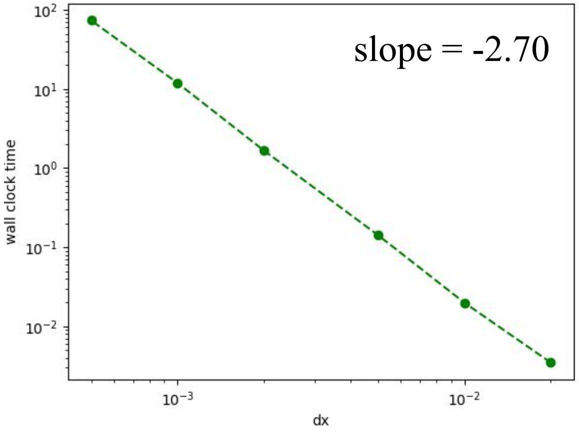
Performance



PCM

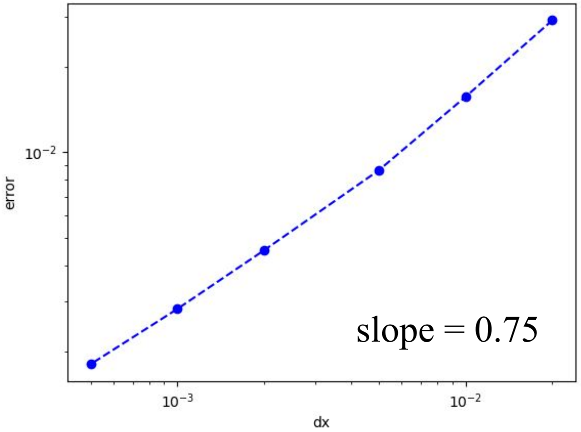


PLM

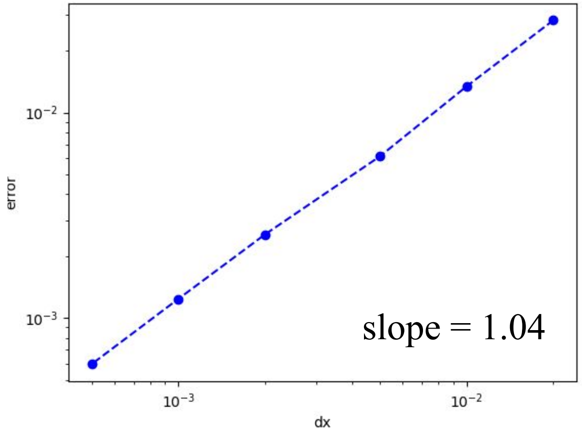


PPM

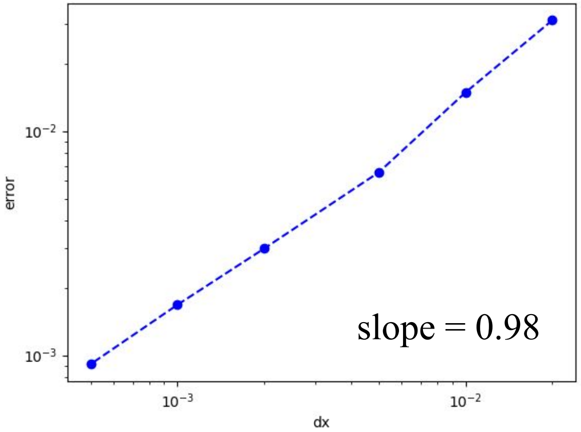
Accuracy (shock tube problem)



PCM



PLM



PPM

Current Problem

- PLM and PPM show only first order accuracy.
- According to Stone et al. (2018), it's probably because of our HLLC Riemann solver. An additional correction term is required to fix it to second order accurate.
- Will it be better with characteristic tracing step?

Characteristic tracing

- Implement the entire section 4.2.3 in Stone et al. (2018).
- Calculate the data on the left and right side of the “interface”, i.e. $\mathbf{w}_{L,i+1/2}$ and $\mathbf{w}_{R,i-1/2}$, instead of $\mathbf{w}_{L,i}$ and $\mathbf{w}_{R,i}$.
- Construct the eigenvalues and eigenvectors of the linearized equations in the primitive variables, use them to obtain the face-centered data.

Characteristic tracing

- Compute the left- and right-interface values using monotonized parabolic interpolation (similar to Colella & Woodward 1984).

$$\hat{\mathbf{w}}_{L,i+1/2} = \mathbf{w}_{R,i} - \lambda^{\max}\frac{\delta t}{2\delta x}\left[\delta\mathbf{w}_i^m - \left(1 - \lambda^{\max}\frac{2\delta t}{3\delta x}\right)\mathbf{w}_{6,i}\right]$$

$$\hat{\mathbf{w}}_{R,i-1/2} = \mathbf{w}_{L,i} + \lambda^{\min}\frac{\delta t}{2\delta x}\left[\delta\mathbf{w}_i^m + \left(1 - \lambda^{\min}\frac{2\delta t}{3\delta x}\right)\mathbf{w}_{6,i}\right]$$

$$\lambda = (v_x - a, v_x, v_x, v_x, v_x + a) \qquad \delta\mathbf{w}_i^m = \mathbf{w}_{R,i} - \mathbf{w}_{L,i}, \qquad \mathbf{w}_{6,i} = 6(\mathbf{w}_i - (\mathbf{w}_{L,i} + \mathbf{w}_{R,i})/2)$$

Characteristic tracing

- Subtract the part of each wave family (characteristics) that does not reach the interface in dt/2.

$$\mathbf{w}_{L,i+1/2} = \hat{\mathbf{w}}_{L,i+1/2} + \sum_{\lambda^\alpha > 0} \left[\mathsf{L}^\alpha \left(A(\delta \mathbf{w}_i^m - \mathbf{w}_{6,i}) + B\mathbf{w}_{6,i} \right) \right] \mathsf{R}^\alpha$$

$$\mathbf{w}_{R,i+1/2} = \hat{\mathbf{w}}_{R,i+1/2} + \sum_{\lambda^\alpha < 0} \left[\mathsf{L}^\alpha \left(C(\delta \mathbf{w}_i^m + \mathbf{w}_{6,i}) + D\mathbf{w}_{6,i} \right) \right] \mathsf{R}^\alpha$$

$$\mathsf{R} = \begin{bmatrix} 1 & 1 & 0 & 0 & 1 \\ -a/\rho & 0 & 0 & 0 & a/\rho \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ a^2 & 0 & 0 & 0 & a^2 \end{bmatrix}$$

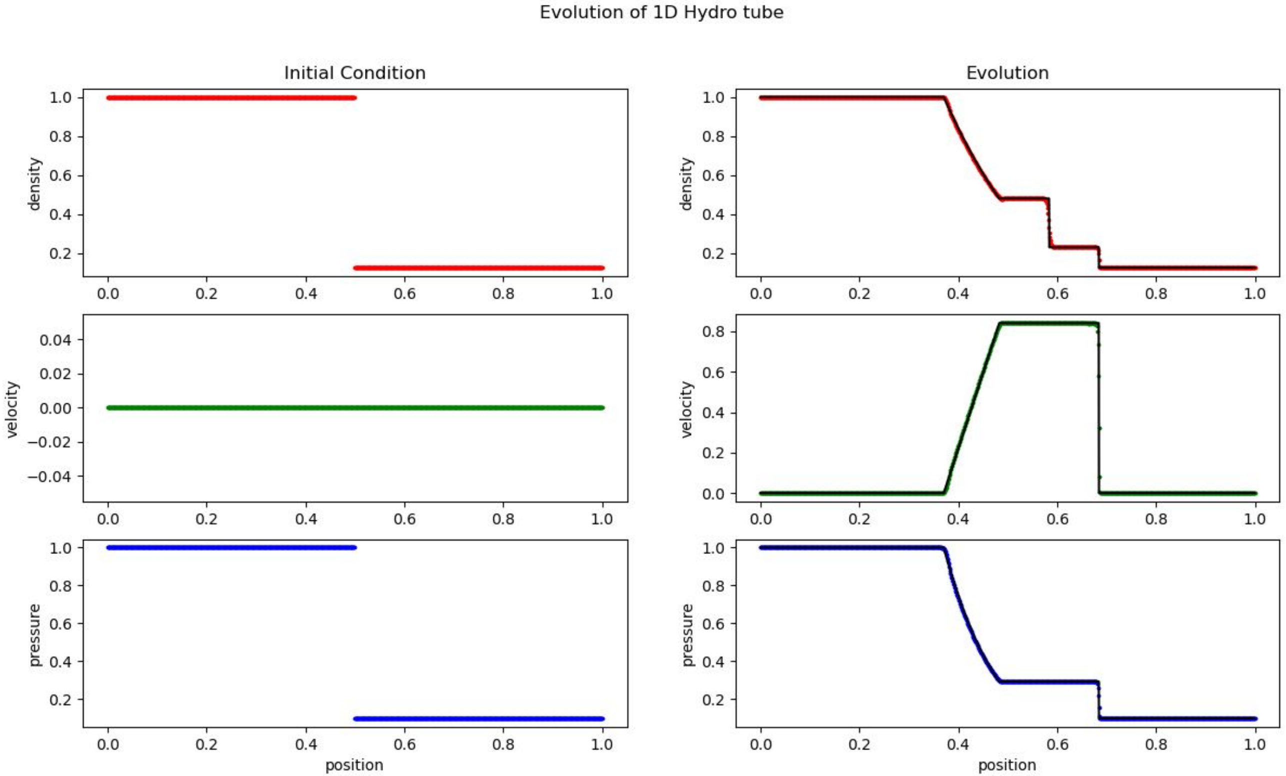
where in the above

$$A = \frac{\delta t}{2\delta x}(\lambda^M - \lambda^\alpha) \qquad B = \frac{1}{3}\left[\frac{\delta t}{\delta x}\right]^2 (\lambda^M \lambda^M - \lambda^\alpha \lambda^\alpha)$$

$$C = \frac{\delta t}{2\delta x}(\lambda^0 - \lambda^\alpha) \qquad D = \frac{1}{3}\left[\frac{\delta t}{\delta x}\right]^2 (\lambda^0 \lambda^0 - \lambda^\alpha \lambda^\alpha)$$

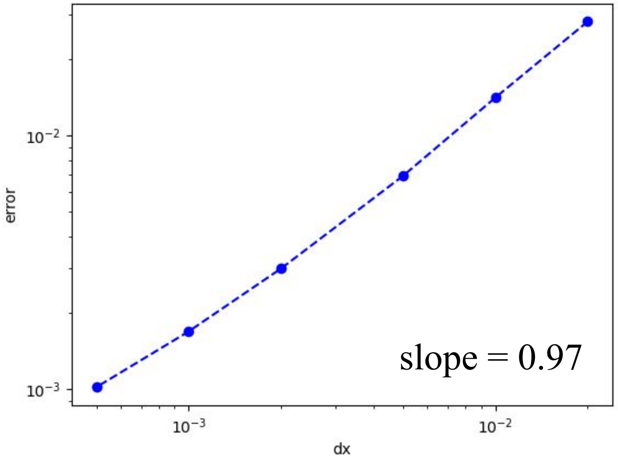
$$\mathsf{L} = \begin{bmatrix} 0 & -\rho/(2a) & 0 & 0 & 1/(2a^2) \\ 1 & 0 & 0 & 0 & -1/a^2 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & \rho/(2a) & 0 & 0 & 1/(2a^2) \end{bmatrix}$$

With characteristic tracing



Characteristic tracing

- Still first order accurate. The result is not better than the original PPM.
- Maybe adding the correction term for HLLC Riemann solver will be better?



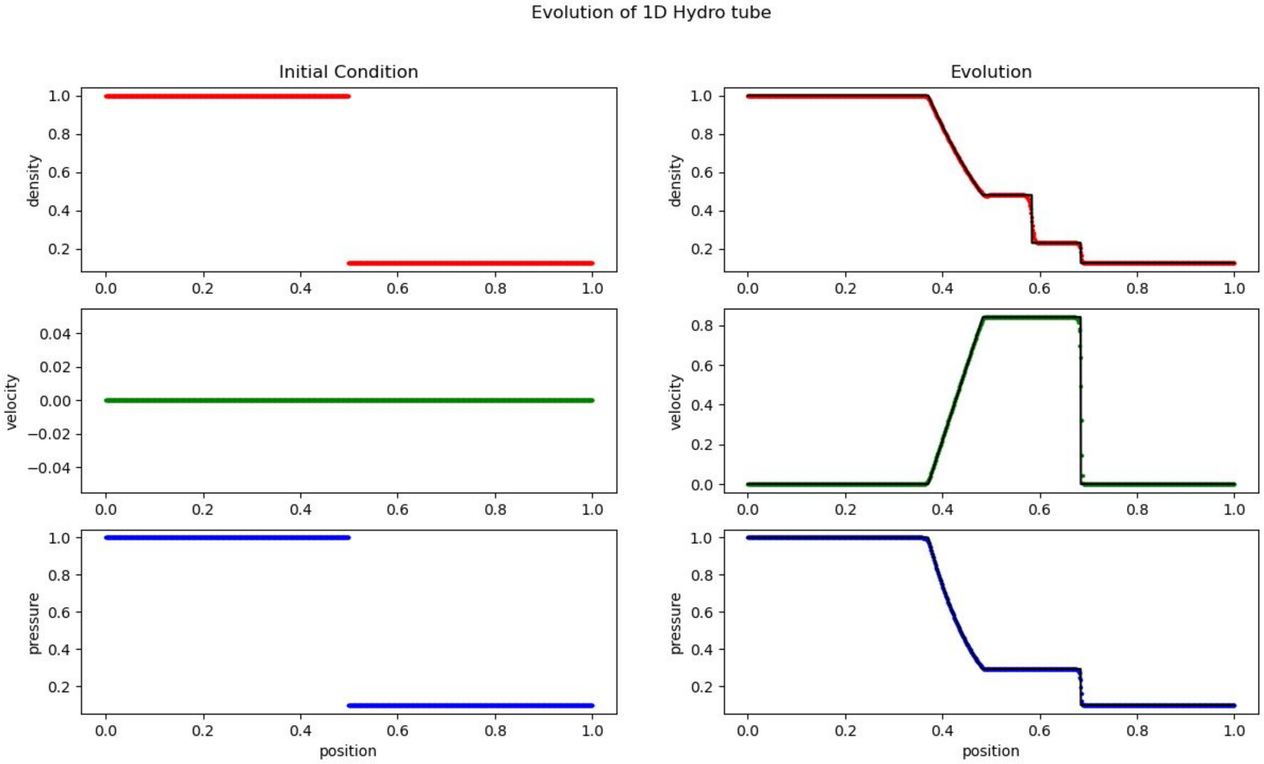
Correction term for HLL family solver

- For approximate Riemann solvers (like HLLC) that average over intermediate states.
- Include a correction for waves which propagate away from the interface in order to make the algorithm higher than first-order.

$$\Delta \mathbf{w}_{L,i+1/2} = -\frac{\delta t}{2\delta x} \sum_{\lambda^\alpha < 0} \left((\lambda_i^\alpha - \lambda_i^M) \mathsf{L}^\alpha \cdot \delta \mathbf{w}_i^m \right) \mathsf{R}^\alpha$$

$$\Delta \mathbf{w}_{R,i-1/2} = -\frac{\delta t}{2\delta x} \sum_{\lambda^\alpha > 0} \left((\lambda_i^\alpha - \lambda_i^0) \mathsf{L}^\alpha \cdot \delta \mathbf{w}_i^m \right) \mathsf{R}^\alpha$$

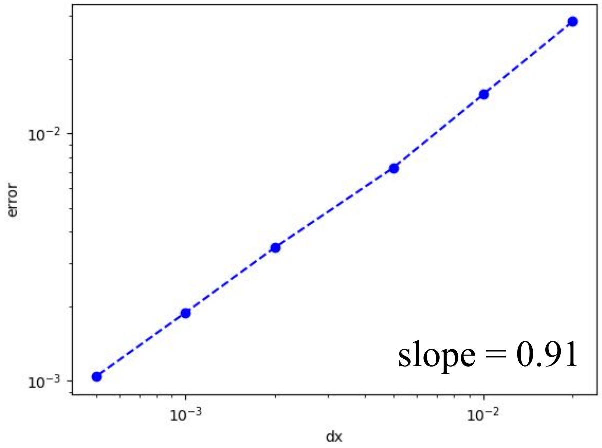
With characteristic tracing + correction



worse???

Characteristic tracing + correction

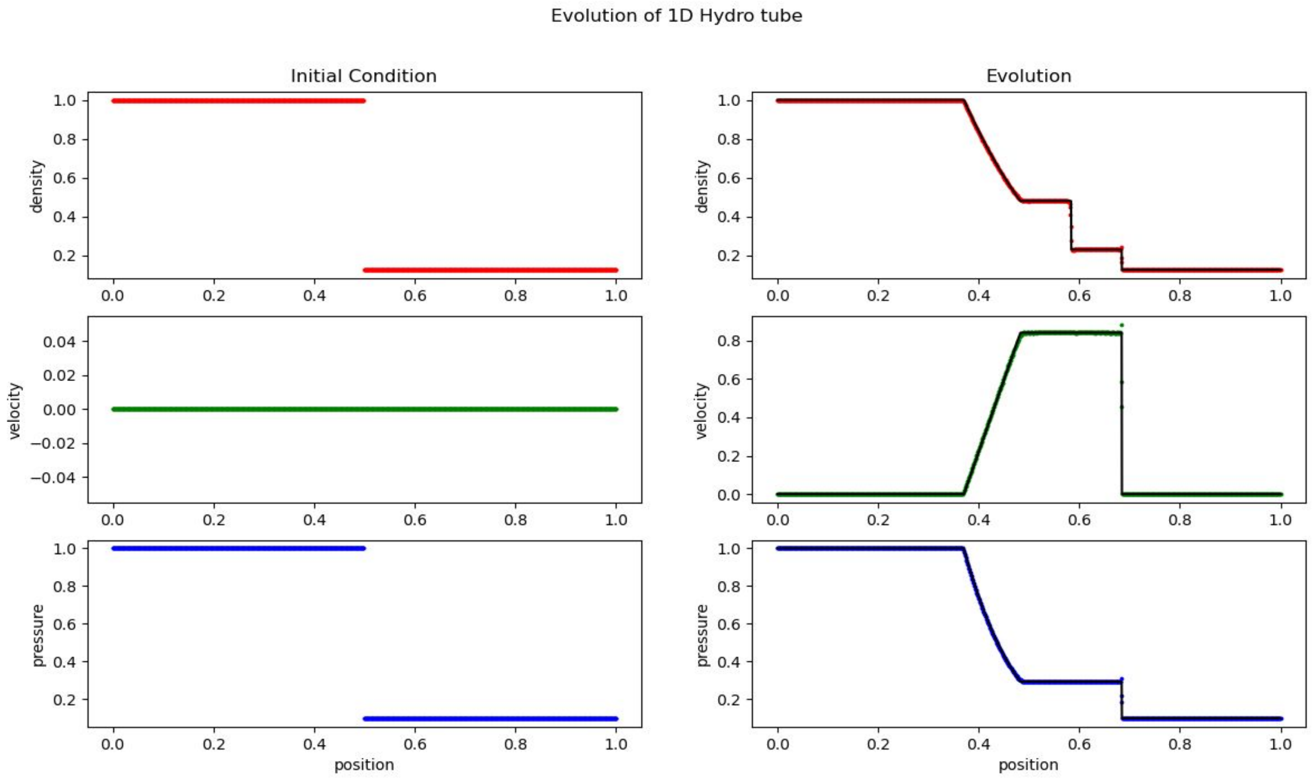
- The correction term doesn’t fix the code to second order accurate.
- Possible reason: bug…?



Another PPM implementation

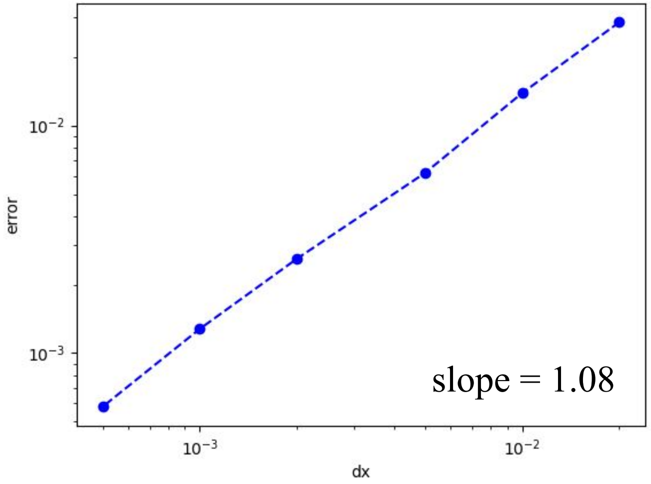
- From section 1 + 3 in the paper of Colella & Woodward (1984).
- Calculate the data on the left and right side of the "interface", i.e. $\mathbf{w}_{L,i+1/2}$ and $\mathbf{w}_{R,i-1/2}$, instead of $\mathbf{w}_{L,i}$ and $\mathbf{w}_{R,i}$.
- Construct the eigenvalues and eigenvectors of the linearized equations in the primitive variables, use them to obtain the face-centered data.
- Should be second order accurate according to the paper.

PPM of Colella & Woodward (1984) result



PPM of Colella & Woodward (1984) result

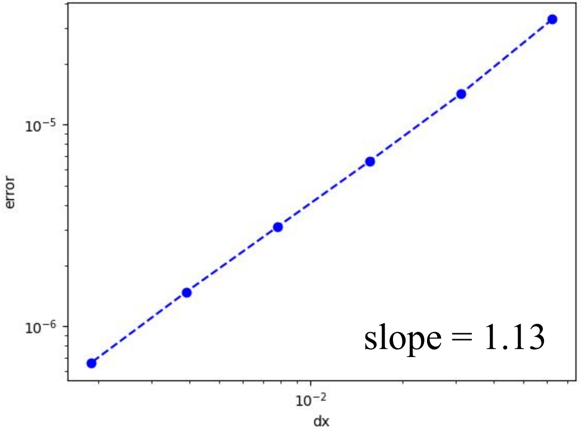
- Can't capture the shock very well. Need further modification.
- This method is first order accurate, too. The error is close to the original PPM method (slightly better).



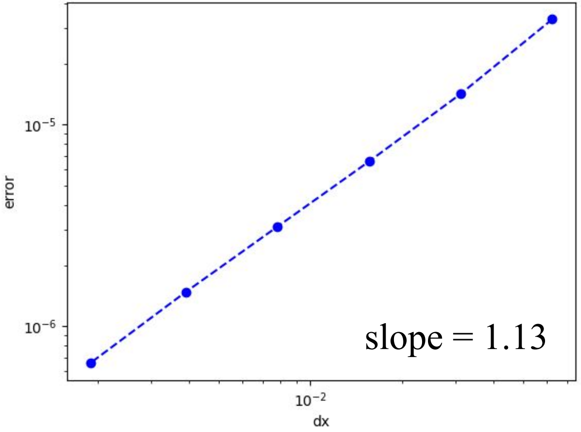
Density error comparison

N	PCM	PLM	PPM	PPM + tracing	PPM + correction	PPM CW
1000	2.815e-3	1.239e-3	1.677e-3	1.687e-3	1.883e-3	1.275e-3
2000	1.799e-3	5.959e-4	9.112e-4	1.015e-3	1.037e-3	5.802e-4

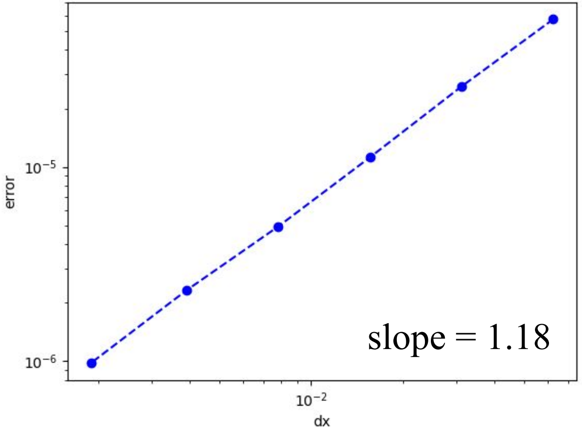
NEW: Accuracy test with acoustic wave problem



PLM



PPM (bug fixed)



PPM with characteristic tracing

Gaussian Process (GP)

Gaussian Process

- Reference: Reyes, A., Lee, D., Graziani, C. et al. A New Class of High-Order Methods for Fluid Dynamics Simulations Using Gaussian Process Modeling: One-Dimensional Case. J Sci Comput 76, 443–480 (2018).
- Use the predictive GP to produce a “data-informed” prediction.

Gaussian Process

Updated posterior mean function:

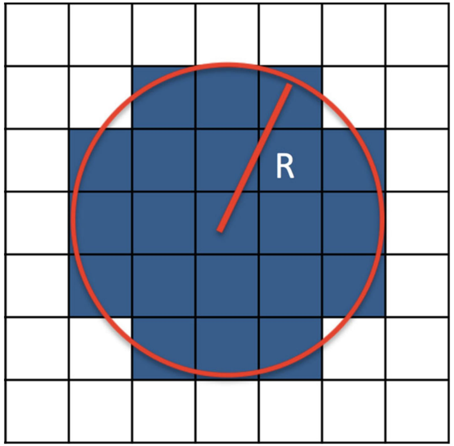
$$\tilde{f}_* \equiv \bar{f}(\mathbf{x}_*) + \mathbf{k}_*^T \mathbf{K}^{-1} \cdot (\mathbf{f} - \bar{\mathbf{f}})$$

$$k_{*,i} = K(\mathbf{x}_*, x_i)$$

$$K(\mathbf{x}, \mathbf{y}) \equiv \Sigma^2 \exp\left[-\frac{(\mathbf{x} - \mathbf{y})^2}{2\ell^2}\right]$$

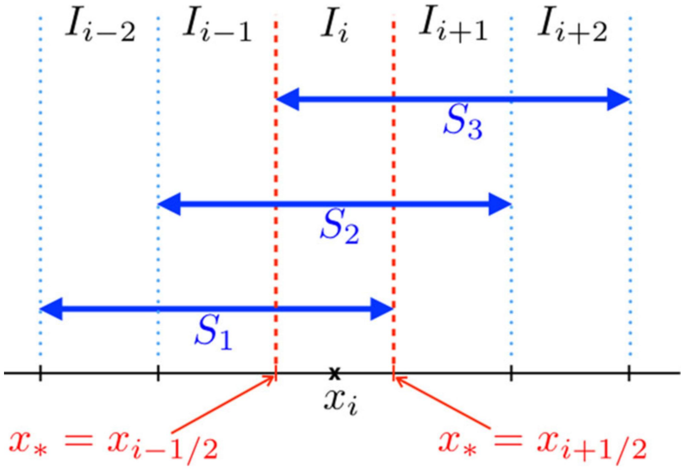
Gaussian Process

- R: stencil radii for Gaussian process
- l: hyperparameter for SE kernel
- Advantage:
    - Directional unbiased reconstriction
    - Solution accuracy can be tuned by kernel hyperparameters



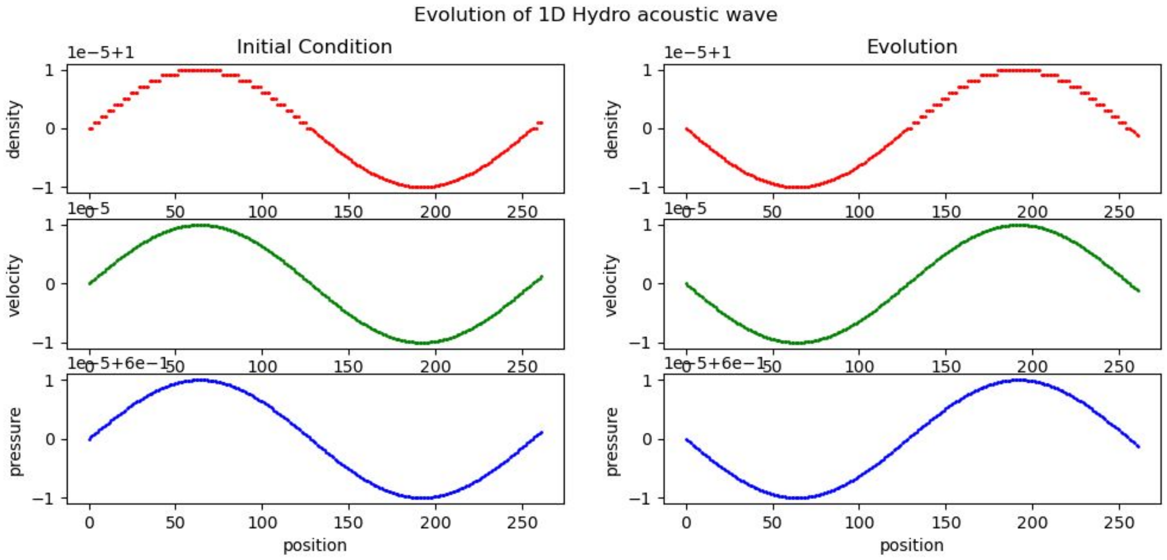
Gaussian Process

- Only applied to smooth wave
- GP-WENO — smooth indicator



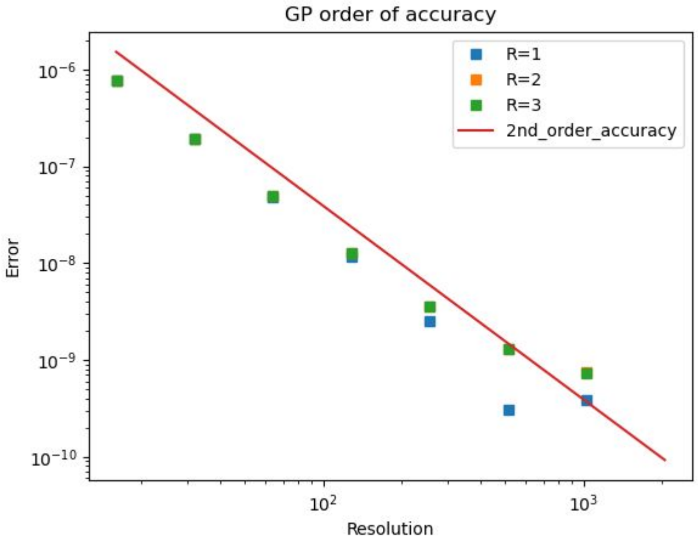
Gaussian Process

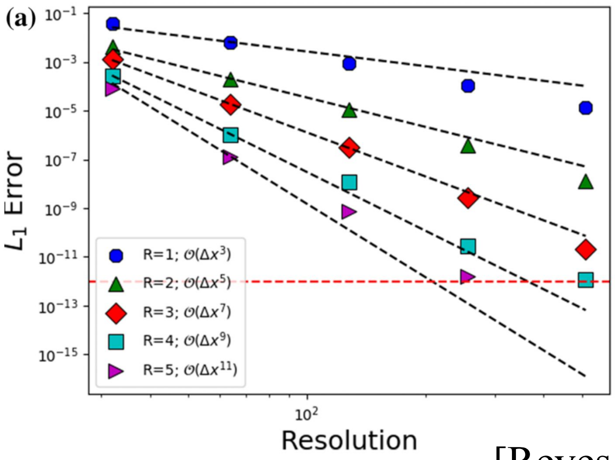
- acoustic wave test



Gaussian Process

- acoustic wave test

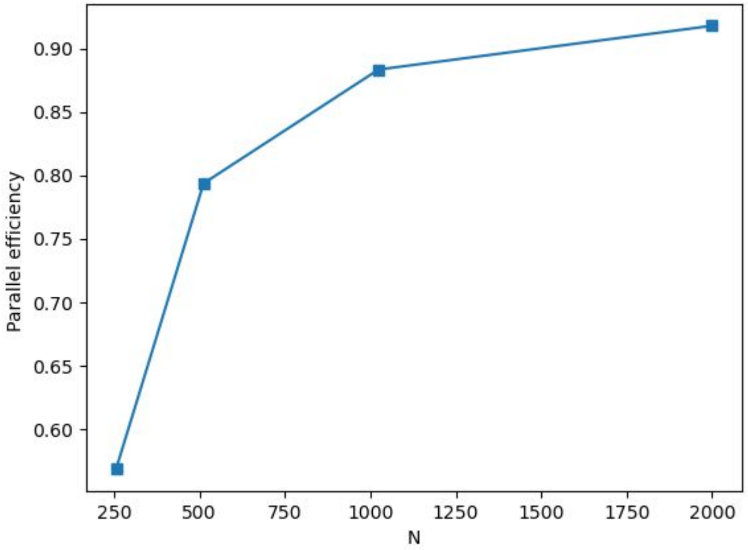




[Reyes 2018]

OpenMP

- Parallel efficiency



Reference

- Colella, P., & Woodward, P.R., 1984. J. Comp. Phys., 54, 174, https://www.sciencedirect.com/science/article/pii/0021999184901438
- Colella, P., & Sekora, M., 2007. J. Comp. Phys, https://www.sciencedirect.com/science/article/pii/S0021999108001435
- Stone et al., ApJS, 178, 137 (2008), https://arxiv.org/abs/0804.0402
- Reyes, A., Lee, D., Graziani, C. et al. J Sci Comput 76, 443–480 (2018). https://doi.org/10.1007/s10915-017-0625-2