Exploring High Order Conservative Finite Difference Methods for Numerical Hydrodynamics using PLUTO Code

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Overview, Motivation & Project Goals

Overview

- This presentation examines advanced numerical techniques for solving hydrodynamic problems using the PLUTO code, focusing on high-order conservative finite difference methods.
- We'll explore the theoretical foundations, implementation in PLUTO, and apply these methods to a range of test cases - from simple 1D shock tubes to complex 2D instabilities - demonstrating their accuracy, efficiency, and robustness in capturing fluid dynamics across various scales and complexities.

Motivation

- The need for high accuracy in complex fluid dynamics simulations crucial for many fields including astrophysics
- The challenges in accurately capturing shocks/discontinuities in fluid flows
- The importance of maintaining conservation properties in numerical schemes to ensure physical validity of the results.

Project Goals

- Understanding PLUTO Code & following the implementation of high-order conservative finite difference methods
- Evaluation of FDM methods' performance across a range of test cases, from simple 1D problems to complex 2D scenarios.
- Testing the accuracy of these methods using L_1 and L_2 norms of errors.
- Preparation of a setup for complex physics which can be used for a more advanced research initiative.

PLUTO Code : Introduction

Purpose and Application:

- A modular, open-source computational code
- Designed for astrophysical hydrodynamics and magnetohydrodynamics.
- Has been used to simulate star formation, accretion disk dynamics etc.

Physics:

- Supports hydrodynamics (HD), magnetohydrodynamics (MHD), relativistic hydrodynamics (RHD), and relativistic MHD (RMHD)

Dimensionality and Grid Configurations:

- The code supports simulations in one, two, and three dimensions
- PLUTO allows for Cartesian, cylindrical, and spherical coordinates

Numerical Methods :

- PLUTO has several advanced numerical schemes to solve PDEs.
- FVM based high-order Godunov-type shock-capturing methods and various Riemann solvers
- It also have Conservative FDM for HD/MHD physics in Cartesian grid.
- Second & Third Order Runge Kutta is used for Time Integrations

PLUTO Code : Code Structure

```
Src
├── Chombo
├── Cooling
│   ├── H2_COOL
│   ├── MINEq
│   ├── Power_Law
│   ├── SNEq
│   └── Tabulated
├── Dust_Fluid
├── EOS
│   ├── Ideal
│   ├── Isothermal
│   ├── PVTE
│   └── Taub
├── Fargo
├── HD
├── Math_Tools
├── MHD
│   ├── CT
│   ├── GLM
│   ├── Hall_MHD
│   ├── Resistivity
│   └── ShearingBox
├── Parallel
├── Particles
├── RHD
├── RMHD
│   └── Radiation
├── States
├── Templates
├── Thermal_Conduction
├── Time_Stepping
└── Viscosity
```

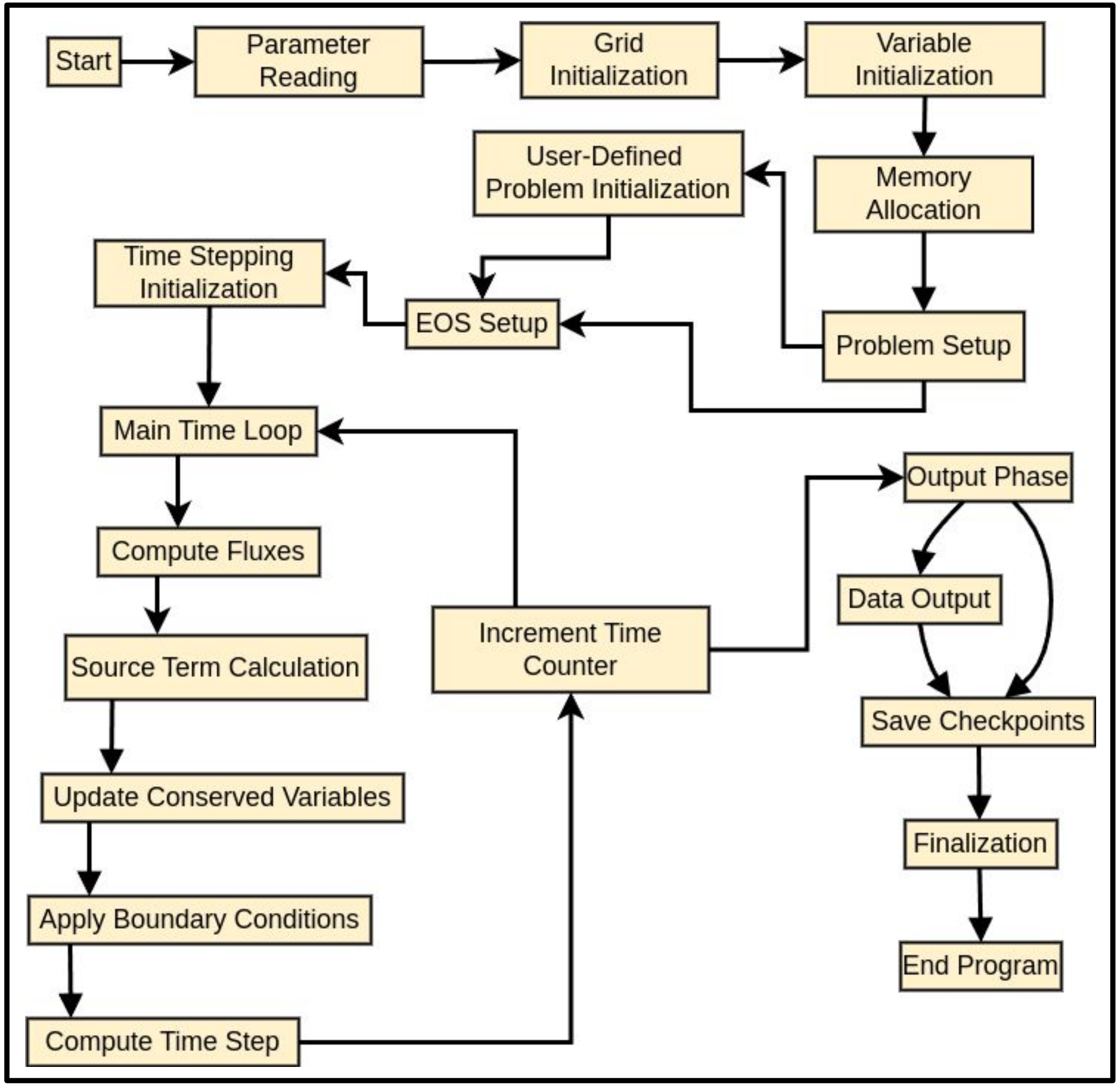
Equation of State related functions

Hydrodynamic Functions like Eigenvector calculation and Primitive to Conservative state calculations

MPI Related Functions

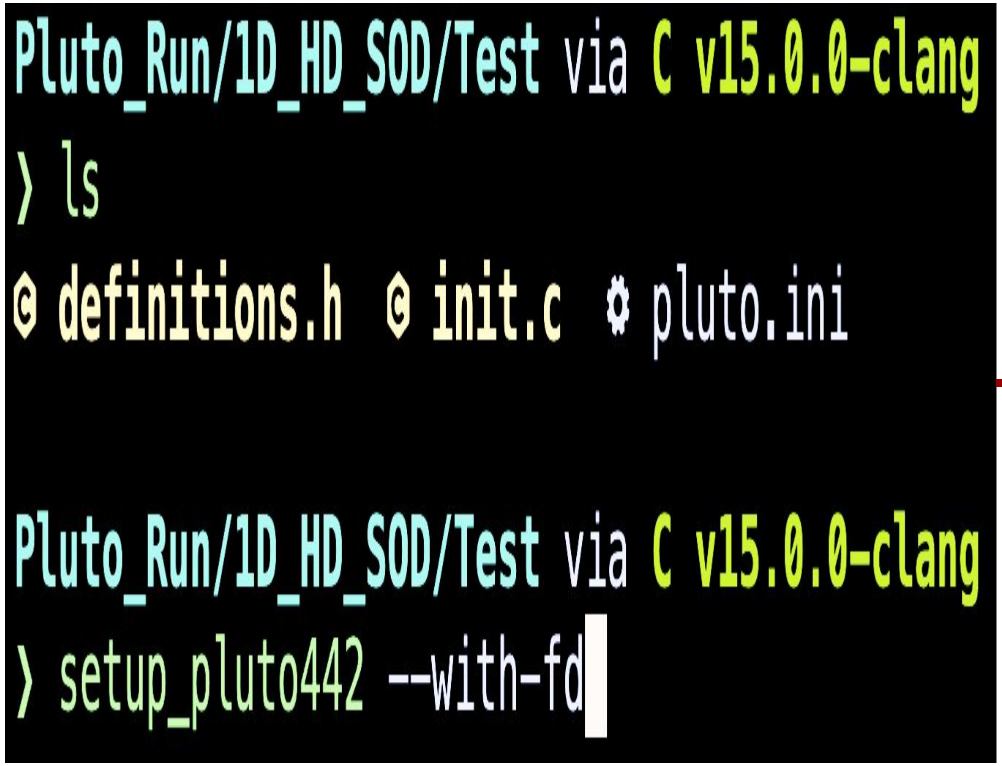
Time-Integration

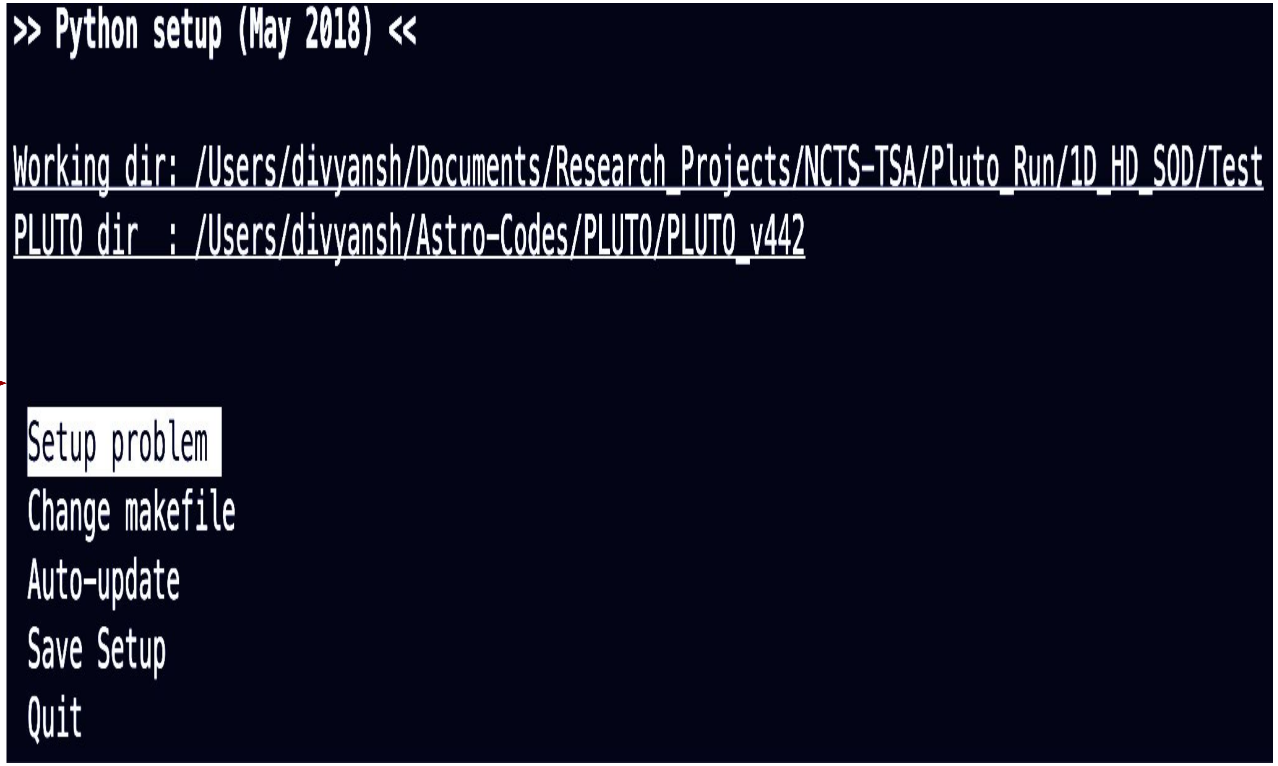
Generic Flowchart of PLUTO Code

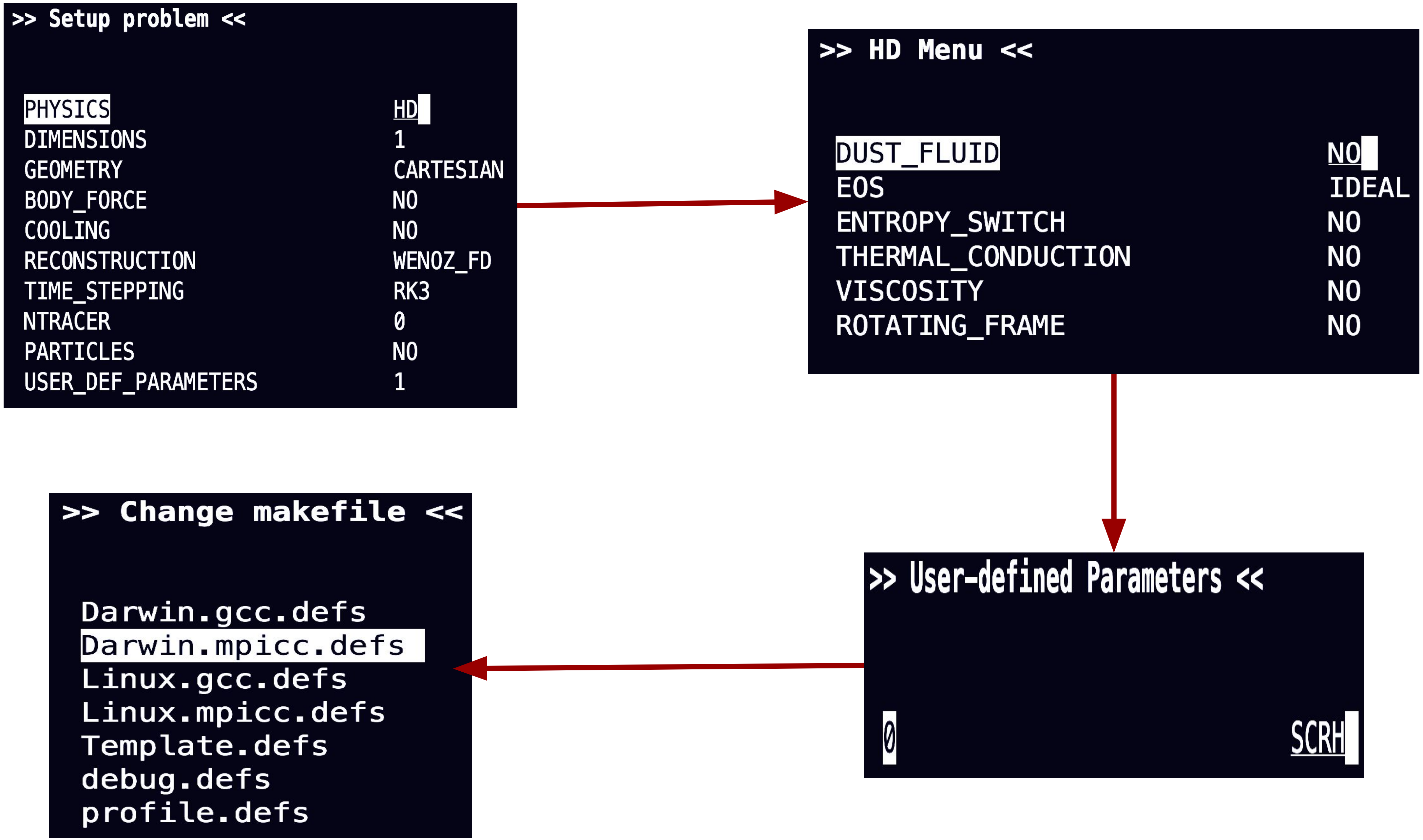


PLUTO Code : Basic Setup

- Copy relevant files from Pluto/Src/Test_Problems/ to your working directory.
- Call the python script and then in the end of generate the makefile.
- Type Make to compile.
- Run the problem with ./pluto or mpiexec -n ./pluto






>> Setup problem <<
PHYSICS HD
DIMENSIONS 1
GEOMETRY CARTESIAN
BODY_FORCE NO
COOLING NO
RECONSTRUCTION WENOZ_FD
TIME_STEPPING RK3
NTRACER 0
PARTICLES NO
USER_DEF_PARAMETERS 1
>> HD Menu <<
DUST_FLUID NO
EOS IDEAL
ENTROPY_SWITCH NO
THERMAL_CONDUCTION NO
VISCOSITY NO
ROTATING_FRAME NO
>> User-defined Parameters <<
0 SCRH
>> Change makefile <<
Darwin.gcc.defs
Darwin.mpicc.defs
Linux.gcc.defs
Linux.mpicc.defs
Template.defs
debug.defs
profile.defs

Conservative FDM for Hydrodynamics

Generic Hyperbolic System in Cartesian coordinate in PLUTO :

$$\frac{\partial \mathbf{U}}{\partial t} = -\sum_{l=x,y,z} \frac{\partial \mathbf{F}_l}{\partial l} + \mathbf{S}$$

$\mathbf{U} =$ Vector holding conservative variables
$\mathbf{F}_l =$ Fluxes in each direction
$\mathbf{S} =$ Vector holding the source terms

Inviscid Hydrodynamics w/o Gravity (No Source Term) :

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho v_z \\ E \end{bmatrix}, \quad \mathbf{F}_x = \begin{bmatrix} \rho v_x \\ \rho v_x^2 + p \\ \rho v_y v_x \\ \rho v_z v_x \\ (E+p) v_x \end{bmatrix}, \quad \mathbf{F}_y = \begin{bmatrix} \rho v_y \\ \rho v_x v_y \\ \rho v_y^2 + p \\ \rho v_z v_y \\ (E+p) v_y \end{bmatrix}, \quad \mathbf{F}_z = \begin{bmatrix} \rho v_z \\ \rho v_x v_z \\ \rho v_y v_z \\ (\rho v_z^2 + p) \\ (E+p) v_z \end{bmatrix}$$

$\rho =$ density
$\mathbf{v} =$ velocity field $= [v_x, v_y, v_z]^T$
$p =$ pressure
$E =$ Total energy $= \frac{p_t}{(\gamma-1)} + \frac{1}{2}\rho\,|\mathbf{v}|^2 = \frac{p_t}{(\gamma-1)} + \frac{1}{2}\rho\left(v_x^2 + v_y^2 + v_z^2\right)$
$\gamma =$ adiabatic index

Conservative FDM for Hydrodynamics

Semi-Discrete Formulation :

$$\frac{d\mathbf{U}}{dt} = \mathcal{L}(\mathbf{U})$$

$$\begin{aligned}\mathcal{L}(\mathbf{U}) = &\ \text{is a high-order approximation to the spatial derivatives} \\ = &-\frac{1}{\Delta x}(\hat{\mathbf{F}}_{x,i+\frac{1}{2},j,k} - \hat{\mathbf{F}}_{x,i-\frac{1}{2},j,k}) - \frac{1}{\Delta y}(\hat{\mathbf{F}}_{y,i,j+\frac{1}{2},k} - \hat{\mathbf{F}}_{y,i,j-\frac{1}{2},k}) - \frac{1}{\Delta z}(\hat{\mathbf{F}}_{z,i,j,k+\frac{1}{2}} - \hat{\mathbf{F}}_{z,i,j,k-\frac{1}{2}})\end{aligned}$$

Third Order Runge-Kutta to Calculate Evolution of Solution from nth Time-Step to (n+1)th :

$$\begin{aligned}\mathbf{U}^{(1)} &= \mathbf{U}^n + \Delta t\mathcal{L}(\mathbf{U}^n) \\ \mathbf{U}^{(2)} &= \frac{3}{4}\mathbf{U}^n + \frac{1}{4}\mathbf{U}^{(1)} + \frac{1}{4}\Delta t\mathcal{L}(\mathbf{U}^{(1)}) \\ \mathbf{U}^{n+1} &= \frac{1}{3}\mathbf{U}^n + \frac{2}{3}\mathbf{U}^{(2)} + \frac{2}{3}\Delta t\mathcal{L}(\mathbf{U}^{(2)})\end{aligned}$$

Conservative FDM for Hydrodynamics

The Interface Flux is computed as :

$$\hat{\mathbf{F}}_{i+\frac{1}{2}} = \sum_j (\hat{V}^{j,+}_{i+\frac{1}{2}} + \hat{V}^{j,-}_{i+\frac{1}{2}}) R^j_{i+\frac{1}{2}}$$

$\hat{V}^{j,\pm}_{i+\frac{1}{2}} = \mathcal{R}(V^{j,\pm}_{i+\frac{1}{2},[s]}) =$ reconstructed characteristic fields

$R^j_{i+\frac{1}{2}} =$ right eigenvectors computed from the conservative field $\mathbf{U}_{i+\frac{1}{2}} = \frac{1}{2}(\mathbf{U}_i + \mathbf{U}_{i+1})$

Characteristic Decomposition :

$$V^{j,\pm}_{i+\frac{1}{2},[s]} = \frac{1}{2}\left(L^j_{i+\frac{1}{2}} \cdot \mathbf{F}_{[s]} \pm \alpha^j \mathbf{U}_{[s]}\right)$$

$L^j_{i+\frac{1}{2}} =$ left eigenvectors of the Jacobian matrix $\partial\mathbf{F}/\partial\mathbf{U}$

$\alpha^j =$ the maximum absolute value of the j^{th} characteristic speed

Conservative FDM for Hydrodynamics

Reconstruction operation :

$$\hat{\phi}_{i+\frac{1}{2}} = \mathcal{R}\left(\phi_{[s]}\right)$$

$$\begin{aligned} \mathcal{R}() &= \text{ a reconstruction operator (WENO-Z or MP5 in this case)} \\ [s] &= \text{ series of points that spans the interpolation stencil} \end{aligned}$$

Currently PLUTO has :

- **2 different 5th order Reconstruction : WENO-Z and MP5**
- **1 3rd order Reconstruction : WENO3**

Conservative FDM for Hydrodynamics

Right and Left eigenvectors of Flux Jacobian :

Defined in ConsEigenvectors Function of PLUTO/Src/HD/eigenv.c file

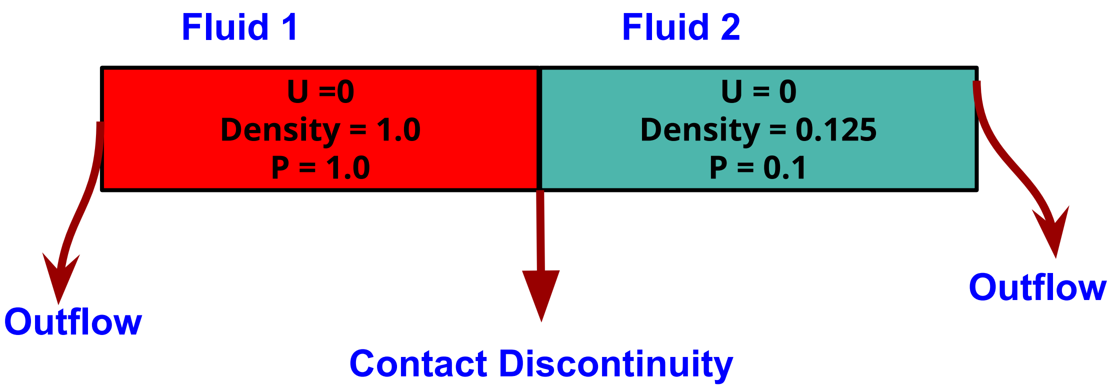
$$\mathbf{R} = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ v_x - a & v_x + a & v_x & 0 & 0 \\ v_y & v_y & v_y & 1 & 0 \\ v_z & v_z & v_z & 0 & 1 \\ H - av_x & H + av_x & \frac{1}{2}(v_x^2 + v_y^2 + v_z^2) & v_y & v_z \end{pmatrix}$$

$$\begin{aligned} \gamma &= \text{ adiabatic index} \\ a &= \text{ speed of sound} \\ H &= \text{ enthalpy } = \frac{1}{2}\left(v_x^2 + v_y^2 + v_z^2\right) + \frac{\gamma p}{(\gamma-1)\rho} \end{aligned}$$

$$\mathbf{L} = \begin{pmatrix} \frac{1}{2}\left(\frac{\gamma-1}{a^2}(H - v_x a) + \frac{v_x}{a}\right) & -\frac{1}{2}\left(\frac{\gamma-1}{a^2}(v_x - a)\right) & -\frac{1}{2}\left(\frac{\gamma-1}{a^2}v_y\right) & -\frac{1}{2}\left(\frac{\gamma-1}{a^2}v_z\right) & \frac{1}{2}\left(\frac{\gamma-1}{a^2}\right) \\ \frac{1}{2}\left(\frac{\gamma-1}{a^2}(H + v_x a) - \frac{v_x}{a}\right) & -\frac{1}{2}\left(\frac{\gamma-1}{a^2}(v_x + a)\right) & -\frac{1}{2}\left(\frac{\gamma-1}{a^2}v_y\right) & -\frac{1}{2}\left(\frac{\gamma-1}{a^2}v_z\right) & \frac{1}{2}\left(\frac{\gamma-1}{a^2}\right) \\ 1 - \frac{\gamma-1}{a^2}\left(v_x^2 + v_y^2 + v_z^2 - H\right) & \frac{\gamma-1}{a^2}v_x & \frac{\gamma-1}{a^2}v_y & \frac{\gamma-1}{a^2}v_z & -\frac{\gamma-1}{a^2} \\ 0 & 0 & 1 & 0 & -v_y \\ 0 & 0 & 0 & 1 & -v_z \end{pmatrix}$$

Validation & Tests : 1D Sod Shock Tube

Reference : Sod, JCP-1978



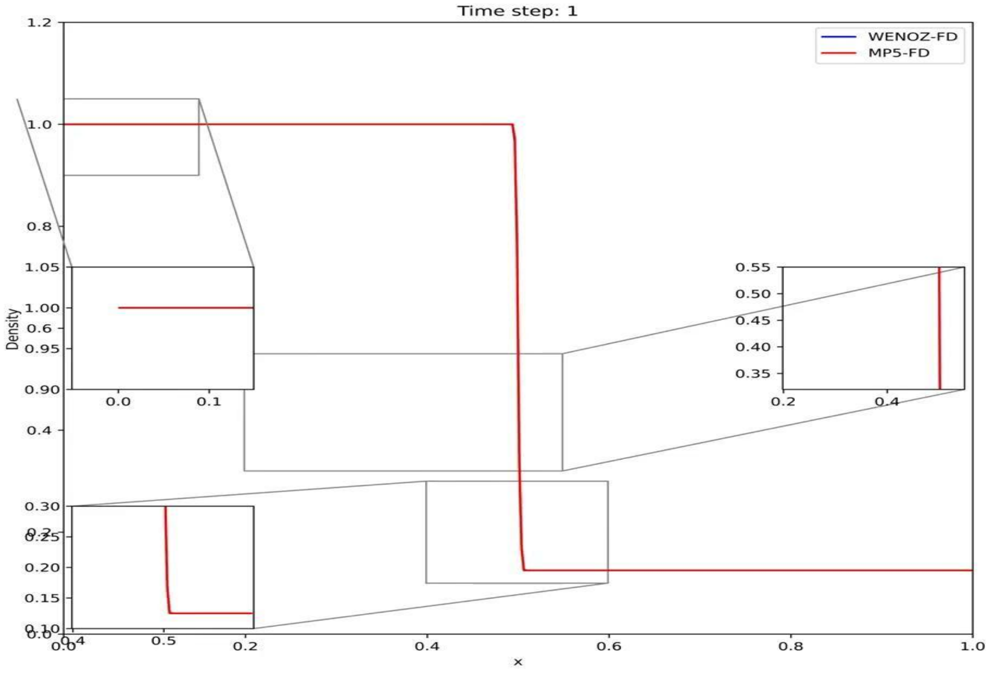
Problem Statement & Overview :

Domain: [$0 \leq x \leq 1$]
Initial Condition in terms of State Variables: (ρ, vx, vy, p) :

- Left state ($x \leq xs$): (1, 0, 0, 1)
- Right state ($x > xs$): (0.125, 0, 0, 0.1)

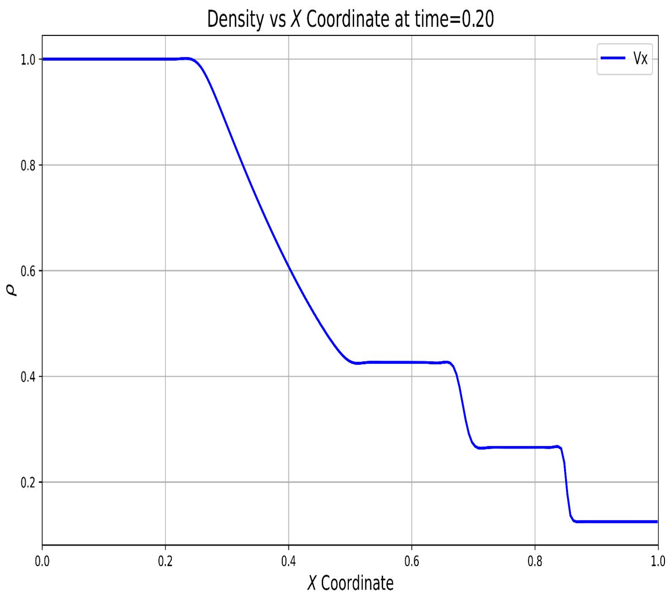
Initial Discontinuity: xs = 0.5
Simulation Parameters: γ (adiabatic index) = 1.4, CFL = 0.4, tmax = 0.2
Results:

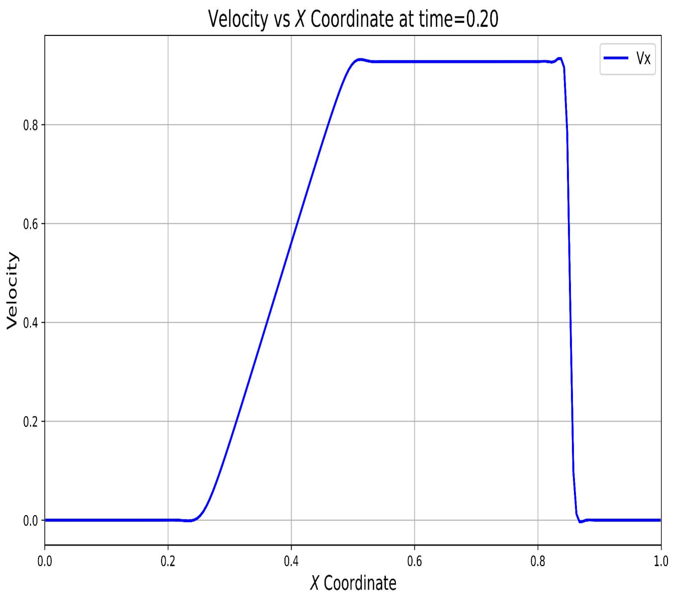
- Solution at t = 0.2 shown
- Captures three key regions:
  1. Left rarefaction
  2. Contact discontinuity
  3. Right shock discontinuity

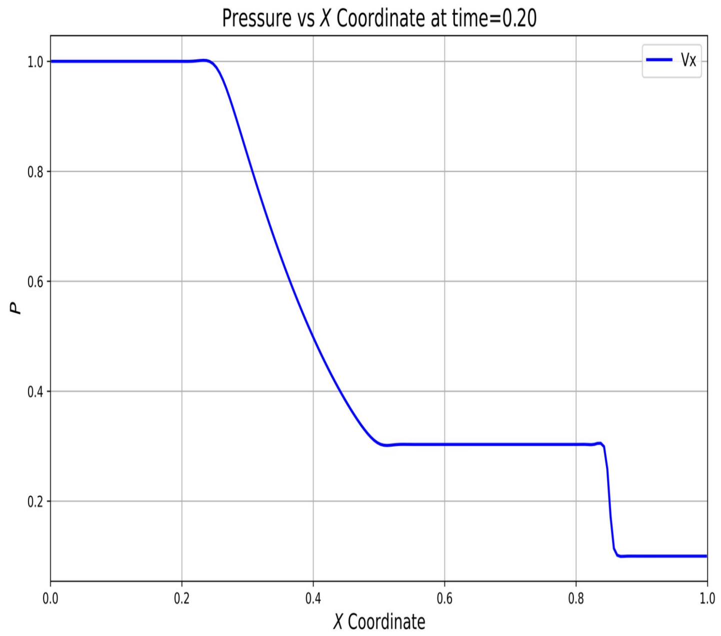


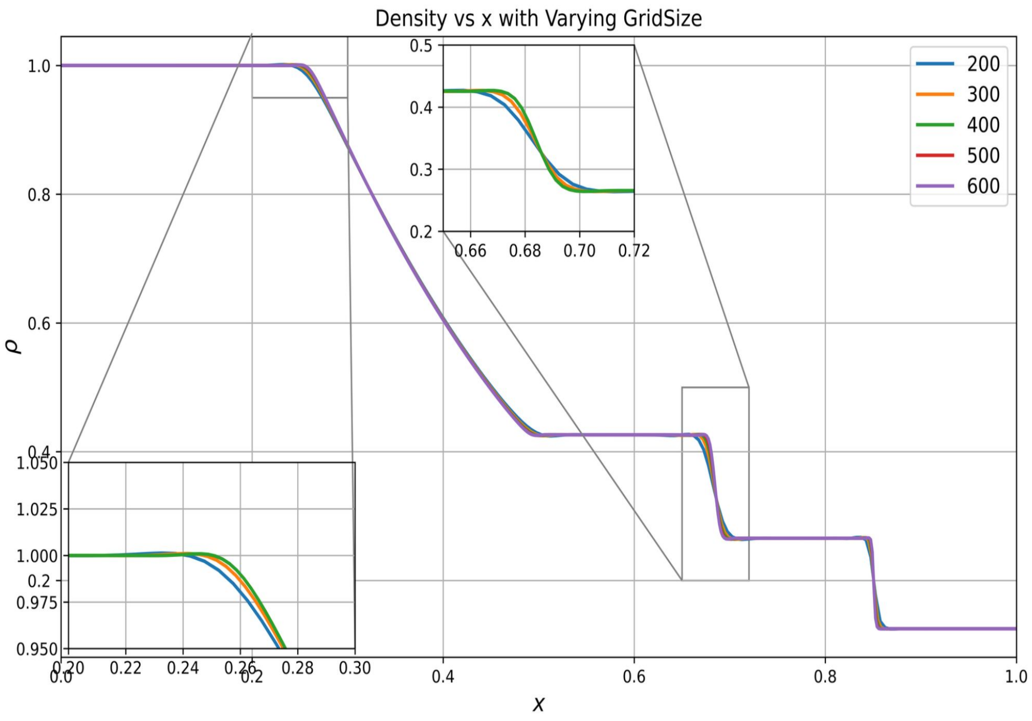
Significance:

- It serves as a basic benchmark for new numerical schemes and codes
- Tests the ability to capture different wave structures simultaneously


Density vs X Coordinate at time=0.20
Vx
ρ
X Coordinate


Velocity vs X Coordinate at time=0.20
Vx
Velocity
X Coordinate


Pressure vs X Coordinate at time=0.20
Vx
P
X Coordinate


Density vs x with Varying GridSize
200
300
400
500
600
ρ
X

Validation & Tests : 1D Shu-Osher Shock Tube

Reference : Shu & Osher, JCP-1988

Problem Statement & Overview :

Domain: [$-5 \leq x \leq 5$]

Initial Condition in terms of State Variables: (ρ, vx, vy, p):

- Left state (x ≤ xs): (3.857143, 2.629369, 0, 10.3333)
- Right state (x > xs): ($1 + A_\rho \sin(f_\rho x)$, 0, 0, 1)
    - A_ρ = 0.2 (density perturbation amplitude)
    - f_ρ = 5.0 (density perturbation frequency)

Initial Discontinuity: xs = -4.0

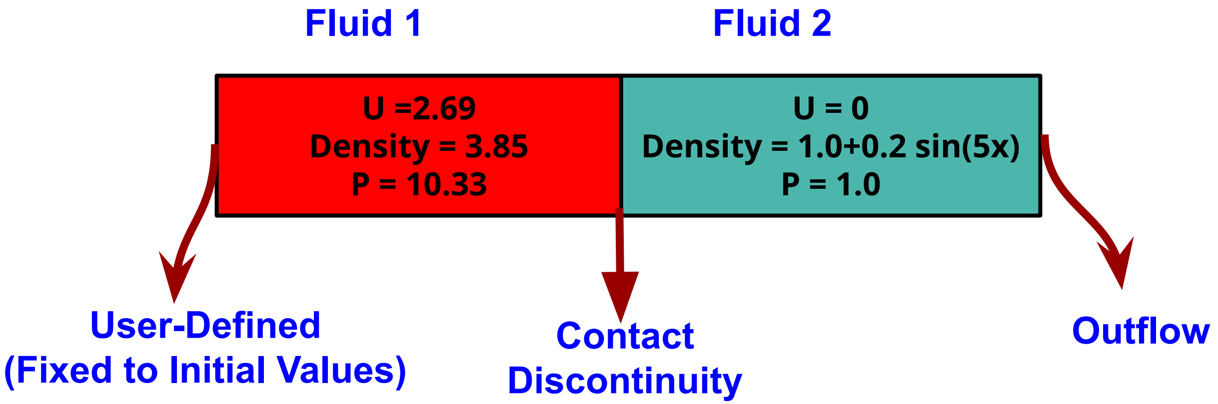
Boundary Conditions:

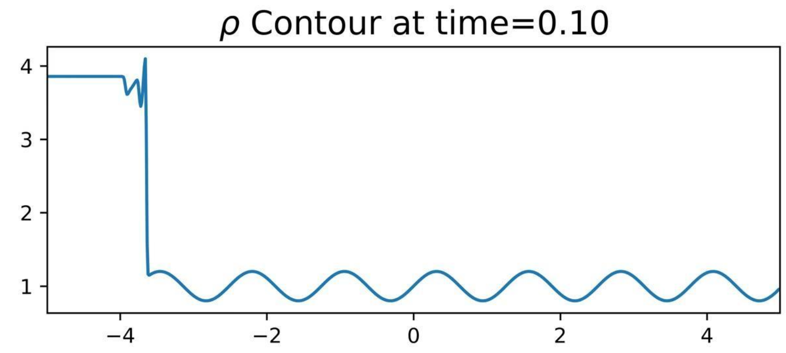
- Left (x = -5): User-defined (Dirichlet, keep Initial values)
- Right (x = 5): Outflow

Simulation Parameters: γ (specific heat ratio) = 1.4, CFL = 0.4, tmax = 1.8

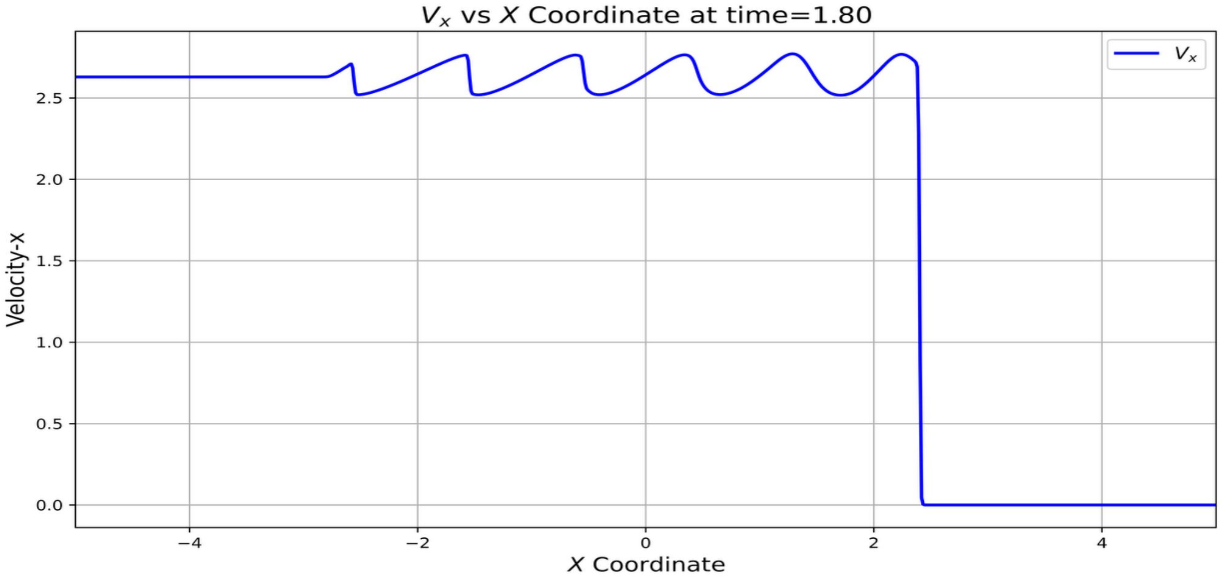
Significance:

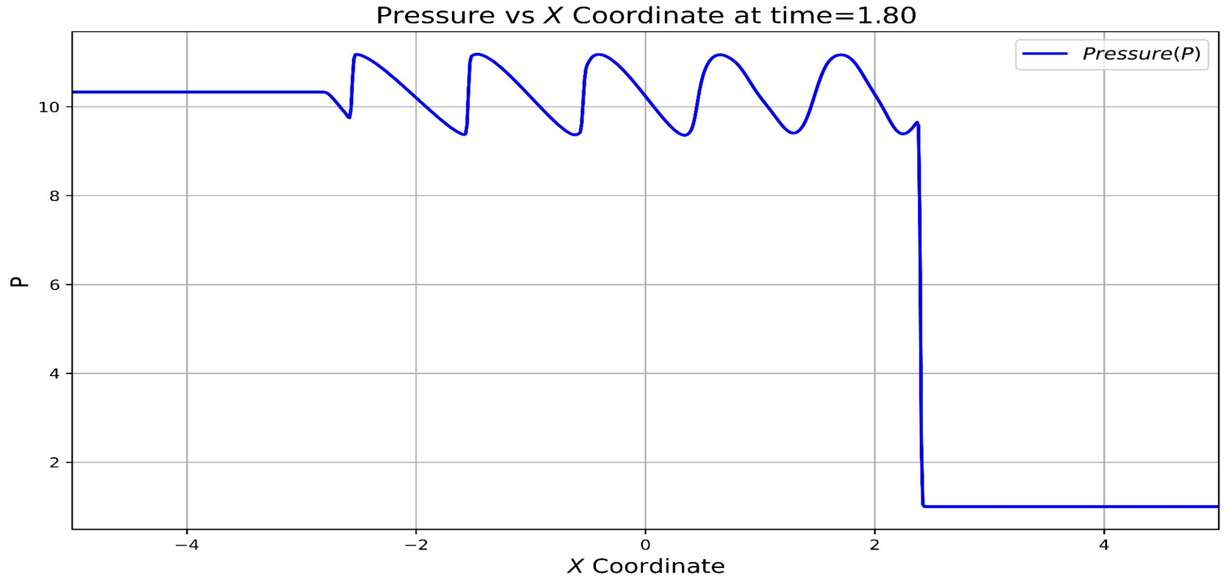
- Helps us to evaluate the performance of high-order methods in resolving the interaction between shocks and entropy waves

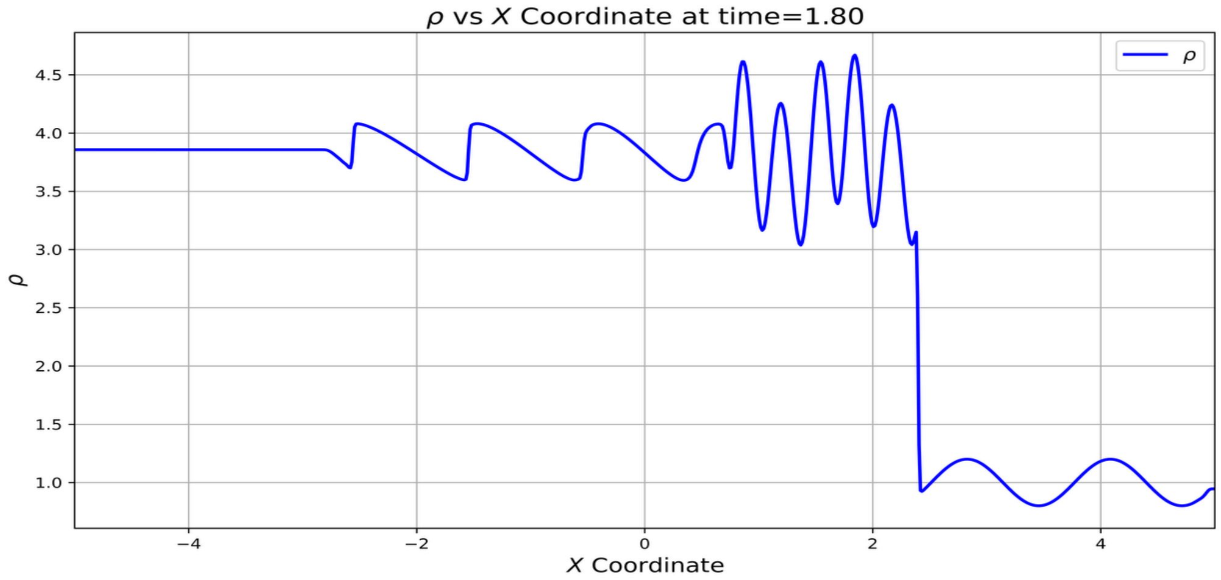




Note : The setup presented here is our own custom setup, PLUTO by default doesn't have this Test


V_x vs X Coordinate at time=1.80
V_x
Velocity-x
0.0
0.5
1.0
1.5
2.0
2.5
−4
−2
0
2
4
X Coordinate


Pressure vs X Coordinate at time=1.80
$Pressure(P)$
P
2
4
6
8
10
−4
−2
0
2
4
X Coordinate


ρ vs X Coordinate at time=1.80
ρ
ρ
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
−4
−2
0
2
4
X Coordinate

Validation & Tests : 2D Isentropic Vortex Advection

Problem Statement & Overview :

Domain: [$0 \leq x \leq 10$, $0 \leq y \leq 10$]
Initial Condition (generic):

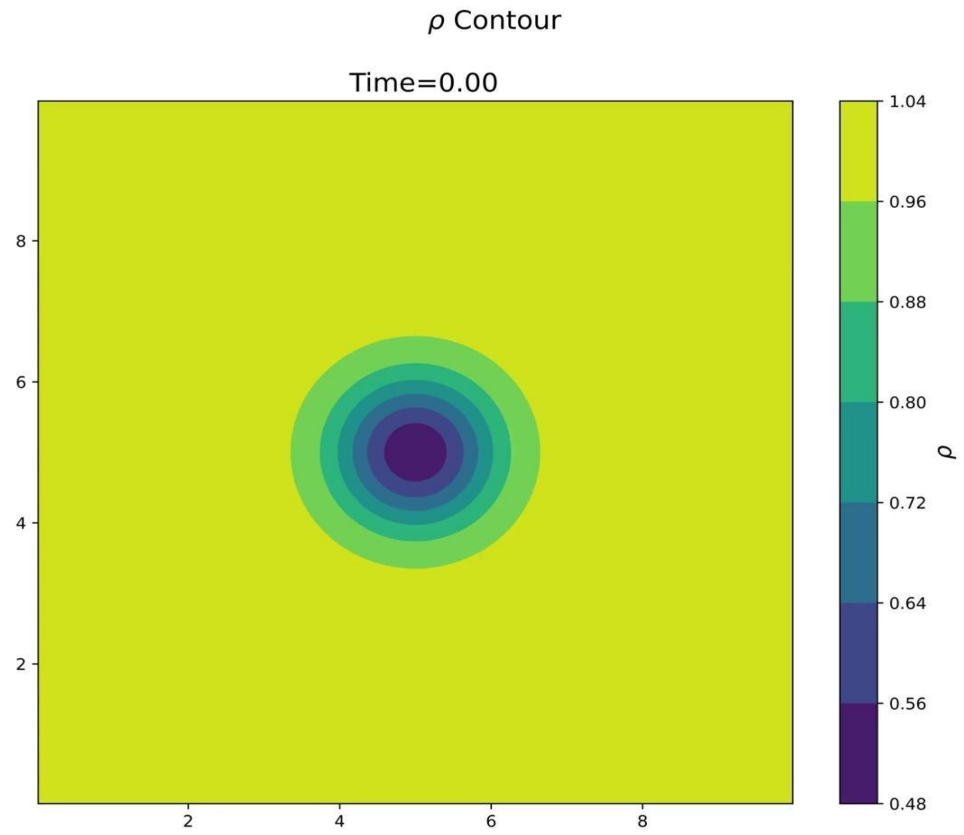
- Velocity perturbations:

  $(\delta v_x, \delta v_y) = -(y_c, x_c) * (\varepsilon/2\pi) * \exp((1-r_c\hat{}2)/2)$

- Temperature: $T = p/\rho = 1 - ((\gamma-1)\varepsilon\hat{}2 / (8\gamma\pi\hat{}2)) * \exp(1-r_c\hat{}2)$
- Entropy: $s = p/(\rho\hat{}\gamma)$
  - ➔ $(x_c, y_c) = (x-5, y-5)$, $r_c = \mathrm{sqrt}(x_c\hat{}2 + y_c\hat{}2)$
  - ➔ ε (vortex strength) = 5, Γ (adiabatic index) = 1.4
  - ➔ Constant entropy s = 1

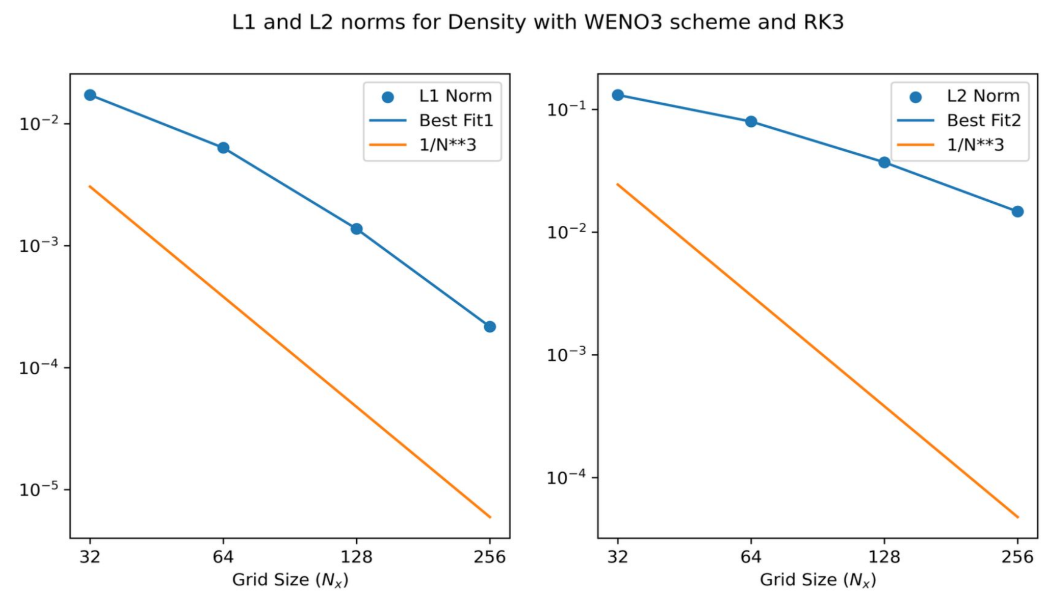
Boundary Conditions: Fully Periodic domain
Vortex Motion:

- Shifts along main diagonal with uniform velocity (1,1)
- Returns to original position after t = 10x structure after several revolutions

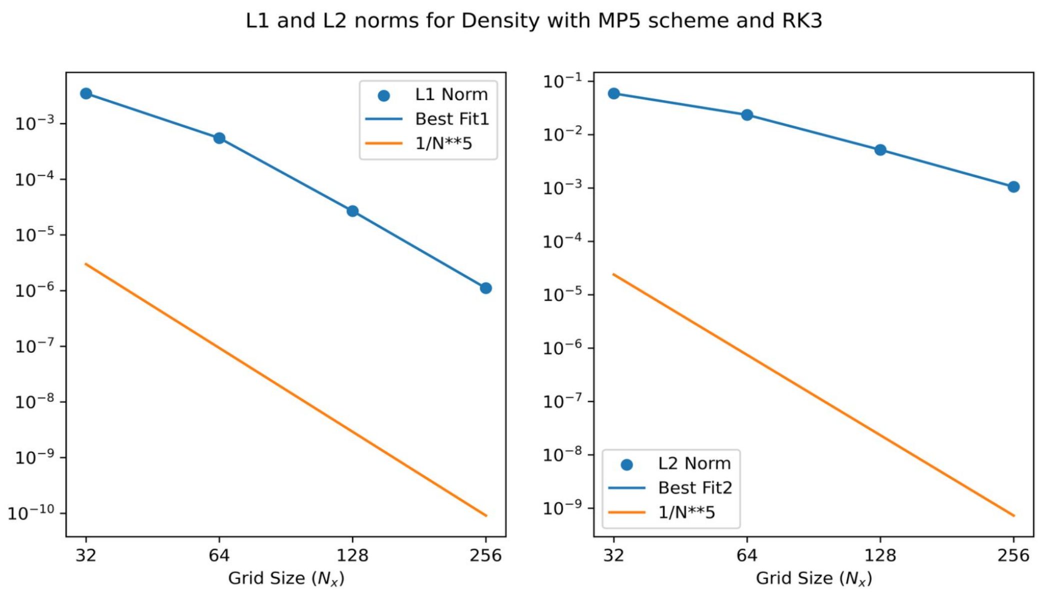


Reference : Shu, 2001, ICASE Report 2001-11

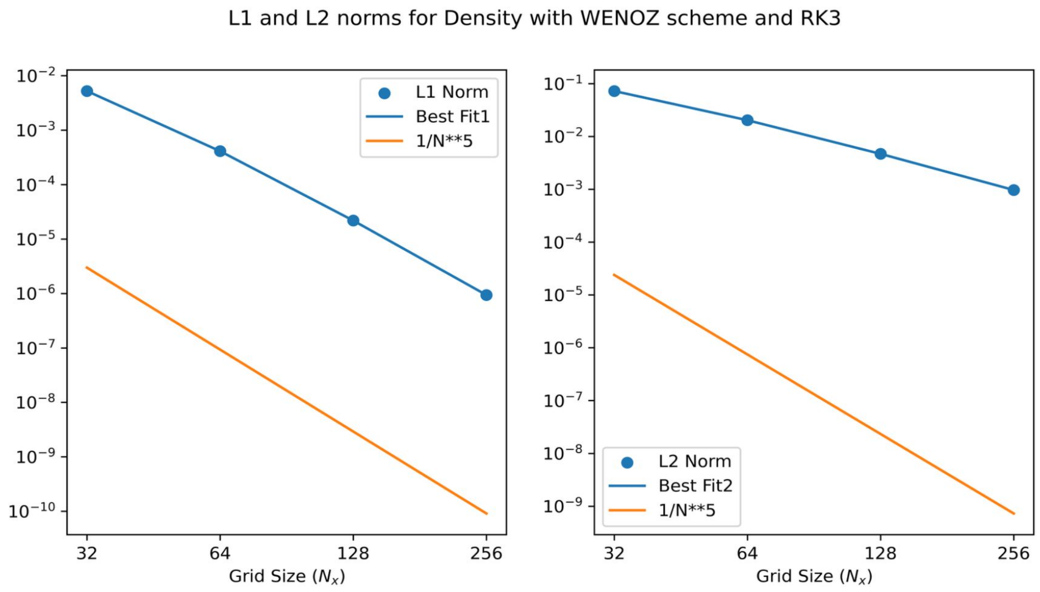
Significance: Computational benchmark for testing accuracy and dissipation of numerical schemes. Evaluates scheme's ability to reproduce vortex structure after several revolutions



L1 and L2 norms for Density with WENO3 scheme and RK3
L1 Norm
Best Fit1
1/N**3
L2 Norm
Best Fit2
1/N**3
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
32
64
128
256
Grid Size (N_x)

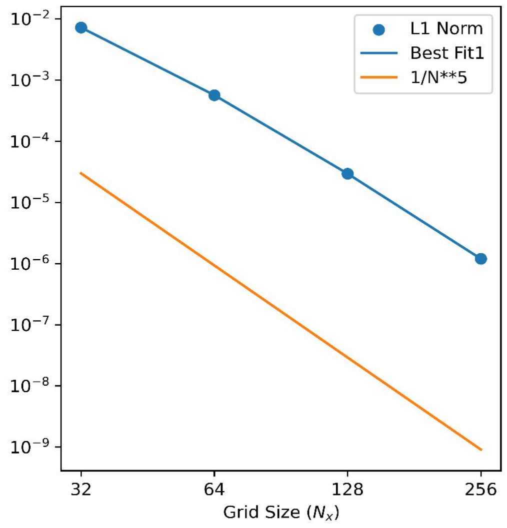


L1 and L2 norms for Density with MP5 scheme and RK3
L1 Norm
Best Fit1
1/N**5
L2 Norm
Best Fit2
1/N**5
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
32
64
128
256
Grid Size (N_x)

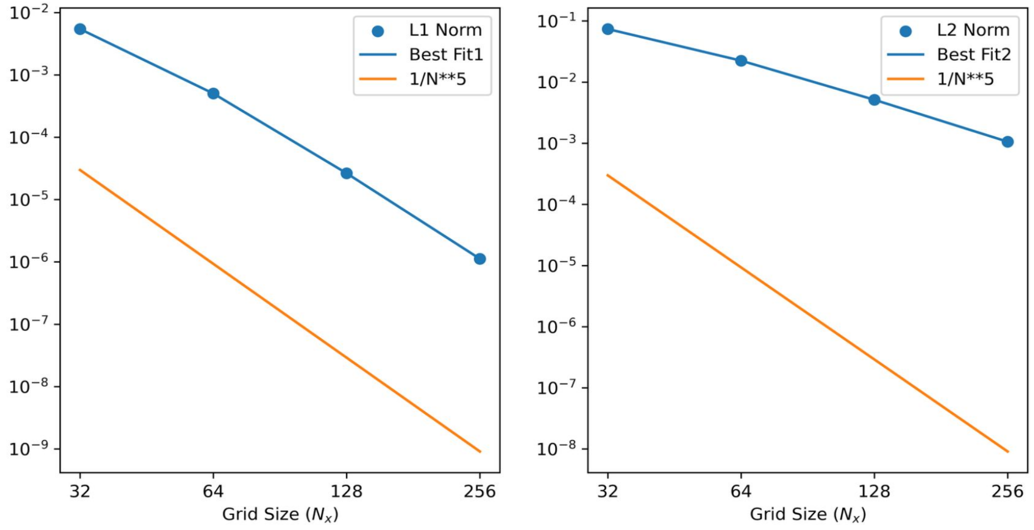


L1 and L2 norms for Density with WENOZ scheme and RK3
L1 Norm
Best Fit1
1/N**5
L2 Norm
Best Fit2
1/N**5
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
32
64
128
256
Grid Size (N_x)

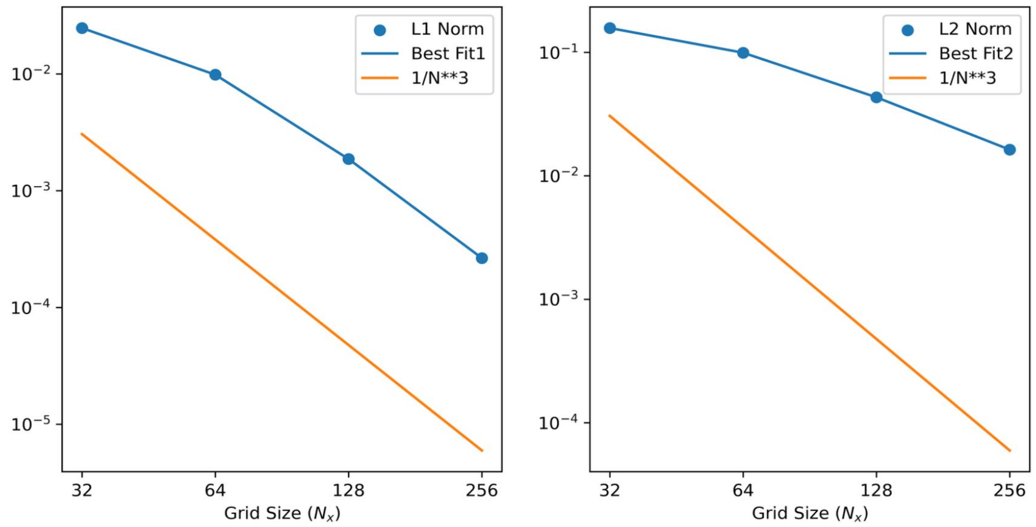
L1 and L2 norms for Pressure with WENOZ scheme and RK3



L1 and L2 norms for Pressure with MP5 scheme and RK3



L1 and L2 norms for Pressure with WENO3 scheme and RK3



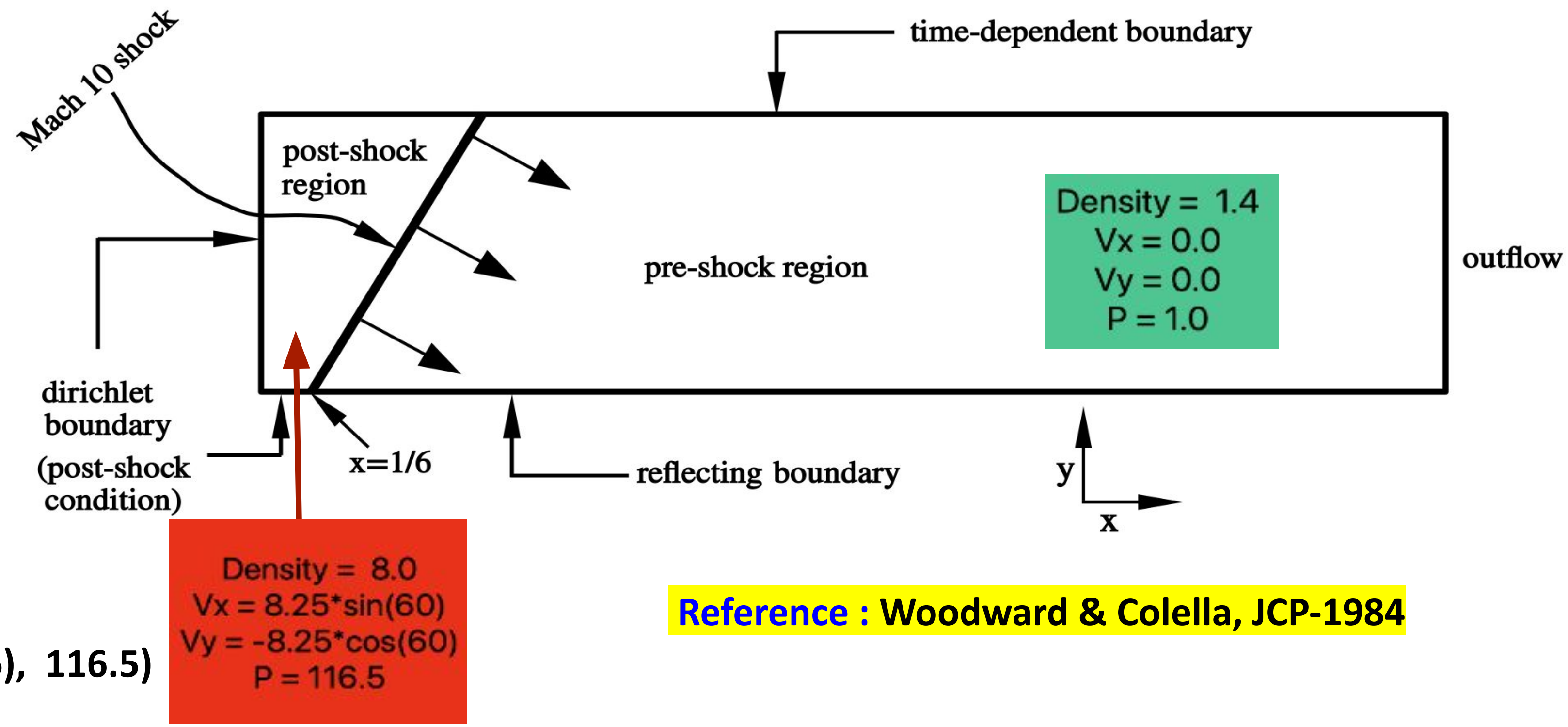
Validation & Tests : 2D Double Mach Reflection

Problem Statement & Overview :

Domain: $[0 \le x \le 4,\ 0 \le y \le 1]$

Initial Condition:

- Mach 10 shock at $x = 1/6$, $y = 0$
- Shock angle: 60° with x-axis
- Plate on bottom from $x = 1/6$



Initial Condition in terms of (ρ, v_x, v_y, p):

- Pre-shock: $(1.4, 0, 0, 1)$
- Post-shock: $(8, 8.25\cos(\pi/6), -8.25\sin(\pi/6), 116.5)$

Reference : Woodward & Colella, JCP-1984

Boundary Conditions:

- Left ($x = 0$): Dirichlet (post-shock state)
- Bottom ($y = 0$): Dirichlet for $0 \le x < ⅙$, Reflecting for $x \ge 1/6$
- Right ($x = 4$): Outflow ($\partial Q/\partial x = 0$)
- Top ($y = 1$): Time-dependent shock position

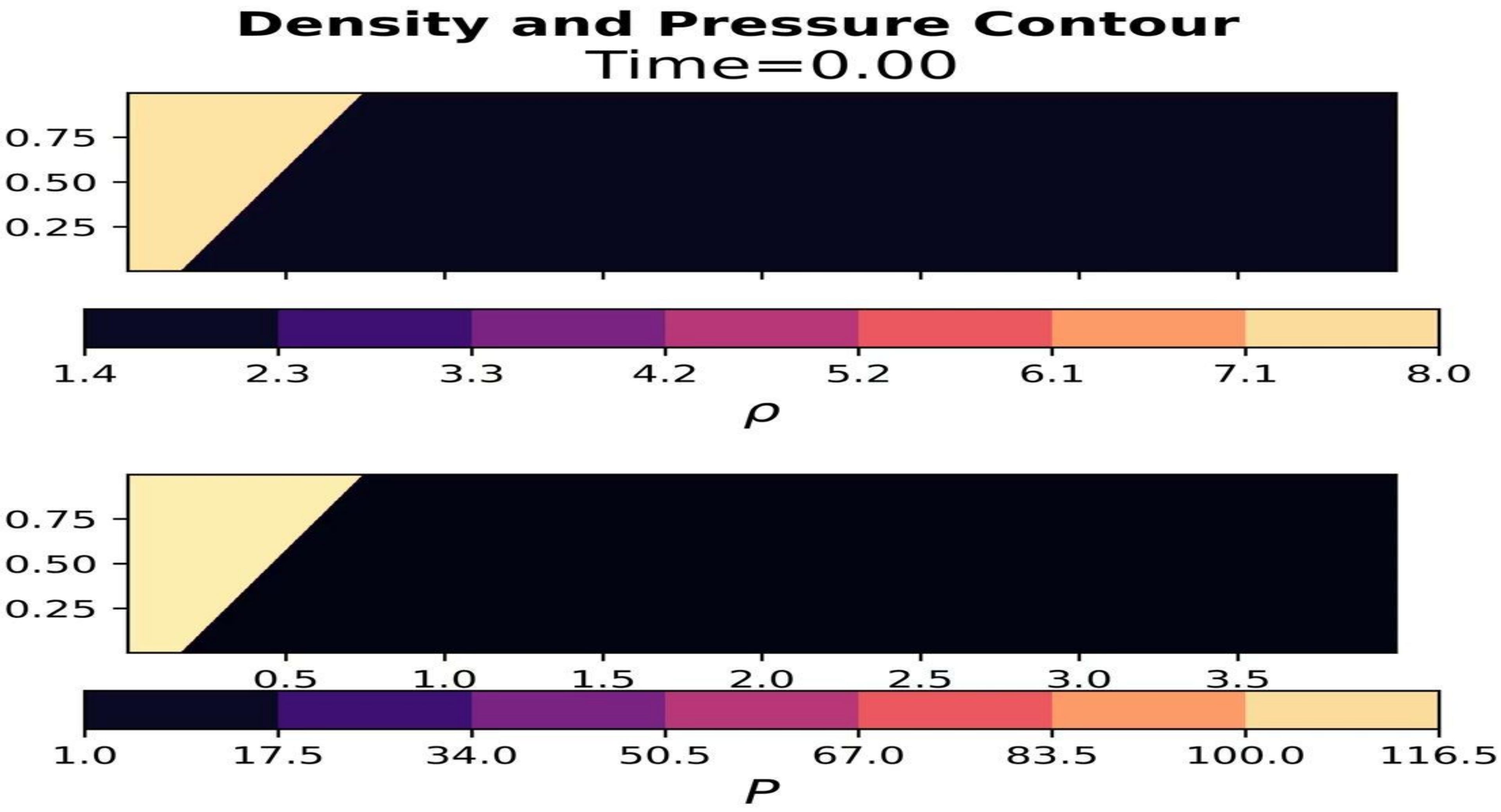
Shock Position at y = 1: $s(t) = x_0 + (1 + 20t)/\sqrt{3}$, where $x_0 = 1/6$

Significance :

- Demonstrates solver's ability to handle complex shock interactions
- Tests accuracy in capturing shock reflections and contact discontinuities
- Challenges numerical schemes with strong gradients and moving discontinuities

Validation & Tests : 2D Double Mach Reflection

Results :



Validation & Tests : Single-Mode Rayleigh Taylor Instability

Problem Statement & Overview :

Domain: [$-0.25 \leq x \leq 0.25$, $-0.75 \leq y \leq 0.75$]

Initial Condition:

- Two layers of the same fluid with different densities
- Heavier fluid on top of lighter fluid
- Hydrostatic equilibrium initially maintained

Density Profile:

- $\rho_1 = 2.0$ for $y > y_0$ (upper layer, heavier)
- $\rho_2 = 1.0$ for $y < y_0$ (lower layer, lighter)
- $y_0 = 0$ is the initial interface position

Pressure Profile:

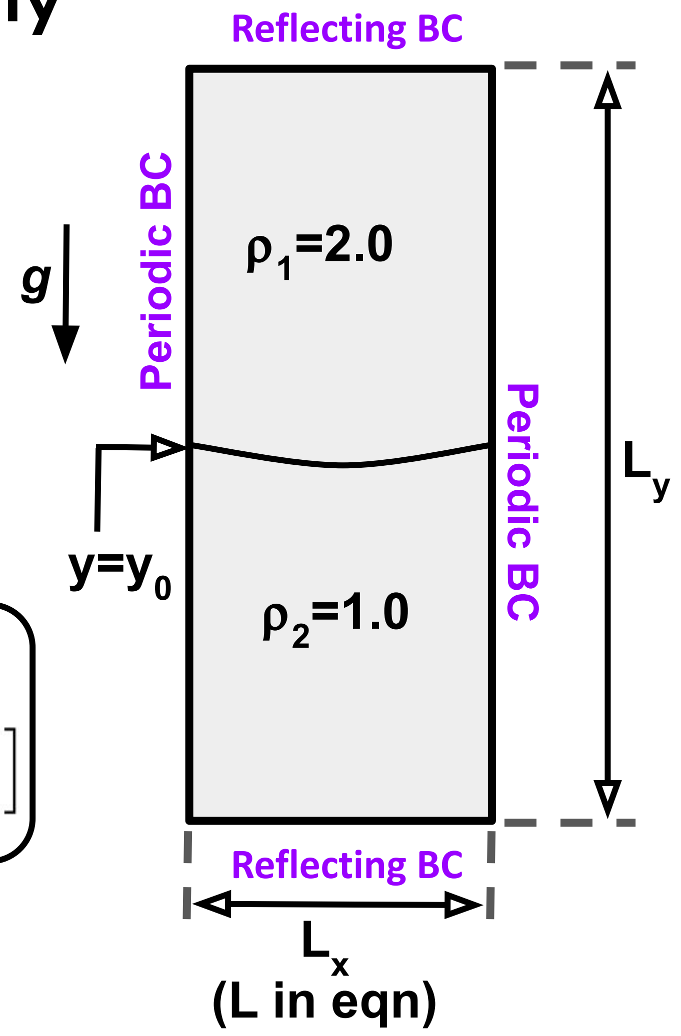
- Continuous across the interface, typically hydrostatic: $dp/dy = -\rho g$

Boundary Conditions:

- $|x| = 0.25 \rightarrow$ Periodic Boundary Conditions
- $|y| = 0.75 \rightarrow$ Reflecting Boundary Conditions

Form of initial perturbation :

$$\frac{A}{2}\left[Cos\left(2\pi K_x \frac{x}{L}\right) + Cos\left(2\pi K_x \frac{x}{L}\right)\right]$$

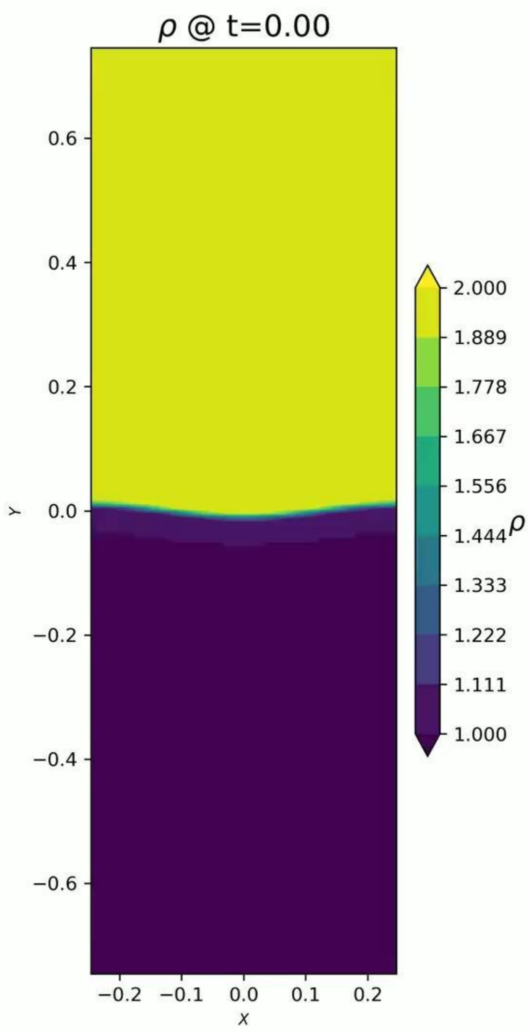


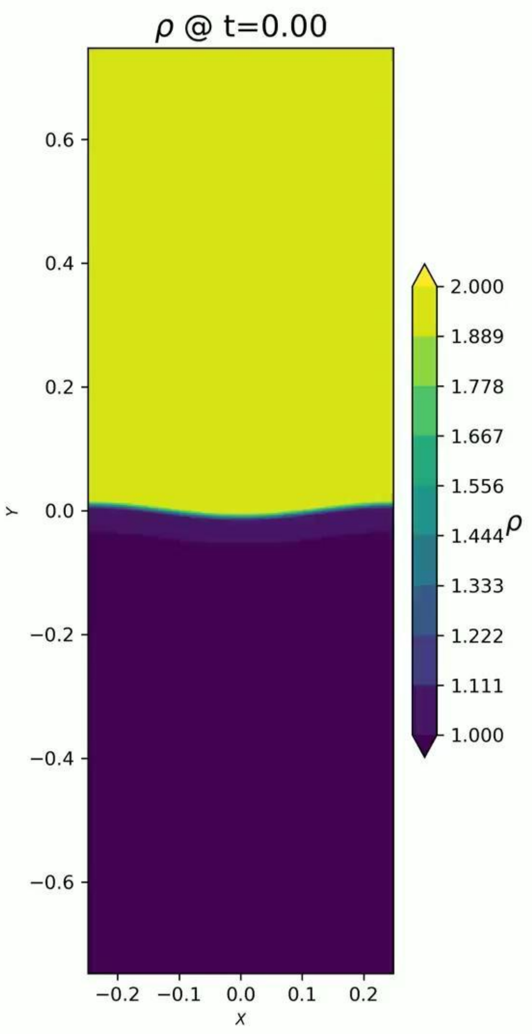
Objective:

- Our aim is to see how disturbance grow at the interface

Validation & Tests : Single-Mode Rayleigh Taylor Instability

Results :





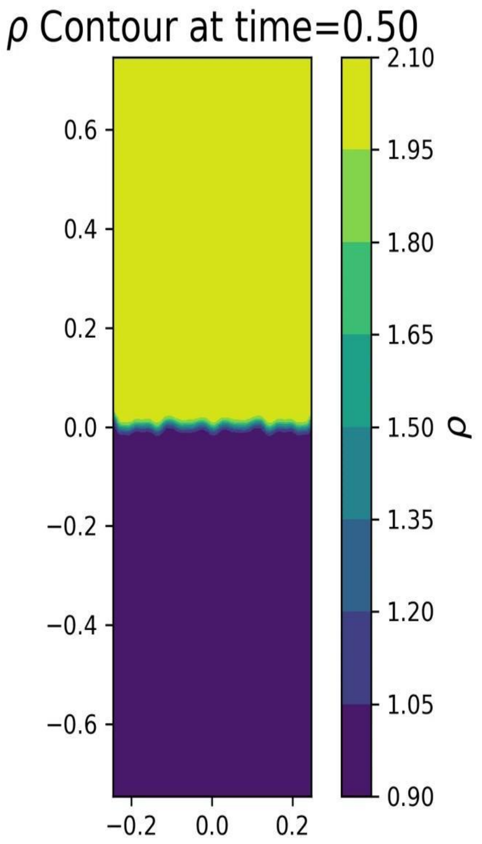
Mesh : 64x192 128x384

- The evolution of density has been presented here
- Early in the simulation (t < 2.0), the differences between low and high resolution is less noticeable.
- The effect of resolution is most prominently visible from t=2.0 as the instability develops and non-linear effects become more pronounced.
- At t=2.3 the mushroom structure between the two solutions have identifiable difference
- Higher resolution is shown to capture:
  - Sharper interfaces between fluids
  - More complex roll-up patterns in the mushroom cap
  - Finer-scale vortices and secondary instabilities
- Low resolution ended up :
  - Smoothing out the mushroom shape
  - Missing smaller-scale features in the cap and stem
  - Failing to resolve secondary instabilities accurately

Complex Setup : Multi-Mode Rayleigh Taylor Instability

Problem Statement & Overview :

- In this perturbations with different modes are given to the liquids.
- Finger like structure are seen forming in form less dense liquid to more dense one.
- The number of finger like structures is directly influenced by the number of modes.



Project Highlights, Remarks & Future Opportunities

Project Highlights :

- Gained comprehensive insight into PLUTO code's versatile capabilities for hydrodynamic simulations
- Developed proficiency in result analysis through specialized post-processing scripts
- Enhanced understanding of numerical code validation techniques through hands-on test cases
- Acquired foundational knowledge of Rayleigh-Taylor Instabilities and their significance in fluid dynamics

Remarks :

- High-order FDM methods show very good accuracy consistent with works done by other researches
- Evidently, PLUTO is very versatile for various hydrodynamic setups, from simple to complex initial condition
- RTI simulations reveal a lot of possible opportunity for studying complex dynamics
- Most of the setup files and post processing script can be found at the advisor’s repository in github :

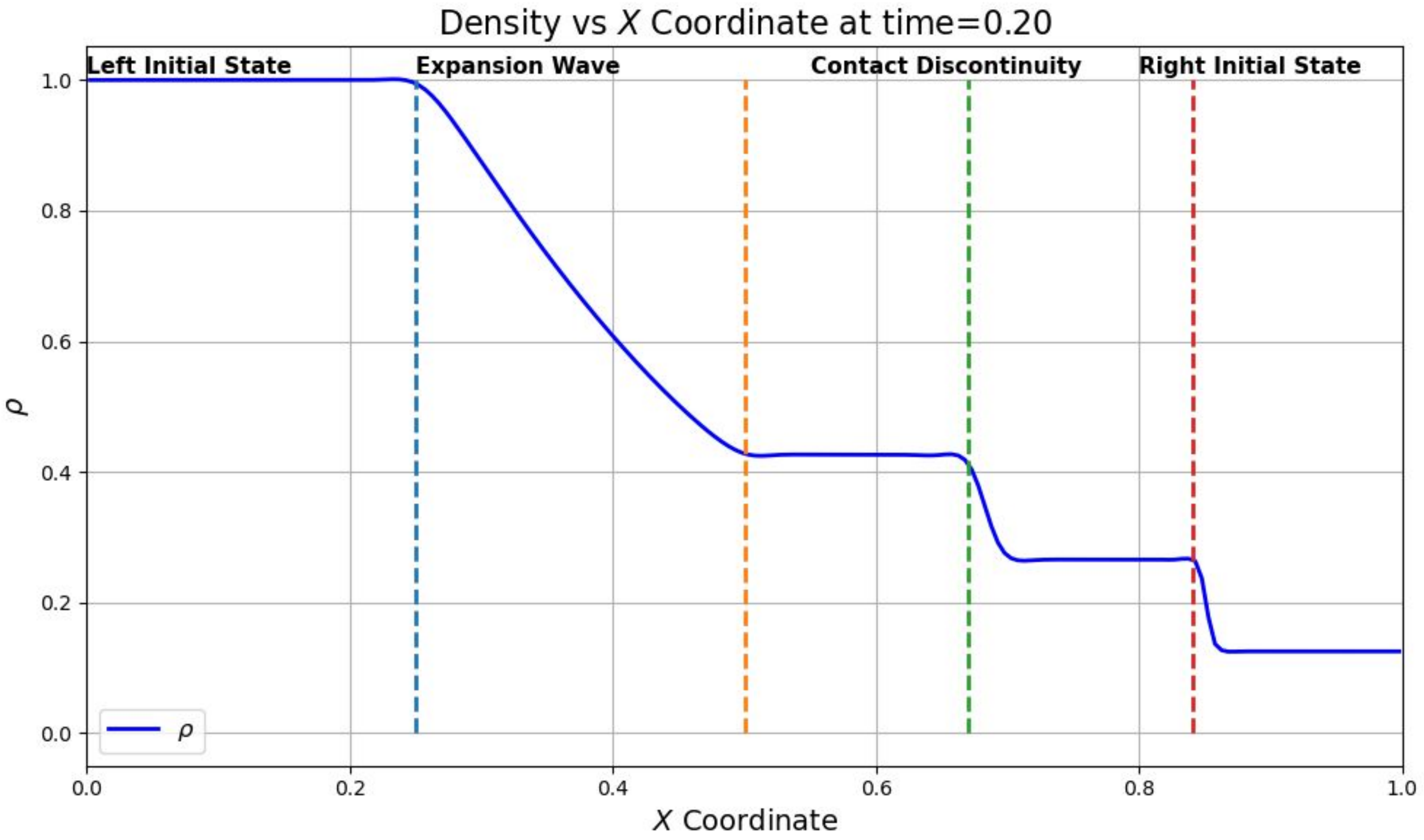
  https://github.com/somdeb1987/StudentProjects/tree/main/ASIAA_SSP-NCTS/2024/Divyansh

Project Highlights, Remarks & Future Opportunities

Future-Opportunities :

- In-depth analysis of mixing layer evolution in the RTI setup
  - Temporal study of mixing layer growth
  - Influence of initial conditions on evolution
  - Comparison with theoretical models
- Detailed analysis of multimode excitation for RTI
  - Examination of mode coupling and interaction
  - Effect on mixing layer structure and growth rate
  - Spectral analysis of multimode perturbations
- Correlation between initial perturbation spectrum and late-time mixing characteristics
- Quantitative assessment of small-scale structures within the mixing layer
- Comparative study of single-mode vs. multimode RTI evolution
- Investigation of transition to turbulence in multimode RTI
- Analysis of energy transfer between different scales in the mixing layer

Thank you


Density vs X Coordinate at time=0.20
Left Initial State
Expansion Wave
Contact Discontinuity
Right Initial State
ρ
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
X Coordinate
ρ