

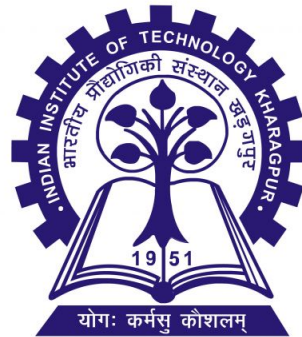
Numerical Schemes for Time Dependent Compressible Euler Equations of Gas Dynamics

Part-I of Bachelor Thesis Project (MA47201)

by

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Under the supervision of
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Literature survey
for part of Bachelor Thesis to be presented at
Indian Institute of Technology, Kharagpur
in partial fulfilment for the degree of
Integrated Master of Science
in
Mathematics and Computing

Declaration

I certify that

- The work contained in this report is not original and has been done by me for learning purposes under the guidance of my supervisor.
- Whenever I have used materials (data, theoretical analysis, figures, and text) from other sources, I have given due credit to them by citing them in the text of the report and giving their details in the references.

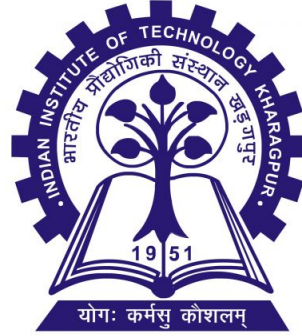
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CERTIFICATE

This is to certify that the Literature survey performed as an initial stage for the Bachelor Thesis Project entitled "**Numerical Schemes for Time Dependent Compressible Euler Equations of Gas Dynamics**" submitted by **Lakshya Bamne (20MA20029)** to Indian Institute of Technology Kharagpur towards partial fulfilment of requirements for the award of degree of Integrated Master of Science in Mathematics and Computing is a record of bona fide work carried out by him under my supervision and guidance during Autumn Semester, 2023-24.

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Abstract

The dynamics of a compressible material¹ (like gases at high pressure situations) is governed by the **Euler equations of gas dynamics**, which is a system of non-linear hyperbolic conservation laws. These high pressure situations are achieved in cases where fluid velocity is above **MACH-1**, which are achieved by supersonic fighter jets and hypersonic space shuttles.

Finding exact solutions for this system of equations is difficult, and in many cases not yet possible. Thus numerical schemes are very important in the fields of Aerodynamics and Fluid Dynamics. Before jumping to solve more complex problems involving the system, we try and develop numerical schemes and test them for **The Riemann Problem**, which is the simplest non-trivial Initial Value Problem for the given system of Partial Differential Equations.

One well established numerical scheme is the *second-order semi-discrete central-upwind (CU) scheme*, which is implemented in this first phase of the project.

All the codes² for this literature survey can be found on the remote github repository: https://github.com/lakshyaBamne/CentralUpwindScheme_1D along with clear instructions to clone the code locally and to reproduce the required results.

Keywords: Compressible Euler Equations for Gas Dynamics, Hyperbolic Partial Differential Equations, Non-linear hyperbolic conservation laws, Second-order semi-discrete central-upwind scheme, Three stage strong stability preserving runge-kutta time discretization, Lax-Friedrichs scheme, Riemann Problems.

¹Here, we neglect the effects of body forces, viscous stresses and heat flux

²codes are in C++ and Python

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Chapter 1

System of Hyperbolic PDE's

1.1 First order PDE's

First order partial differential equations help in understanding several problems concerned with science and technology. They are used in calculus of variations, in the construction of characteristic surfaces for hyperbolic partial differential equations, etc.

In 1-dimensional time dependent case, we have two independent variables and thus the general form of a PDE is as follows,

$$F(x, t, u, u_x, u_t) = 0 \quad (1.1)$$

This is a very general form and we can impose some conditions to deal with some special forms,

1.1.1 Classification for First order PDE's

1. Linear first order PDE (every term is linear in u, u_t, u_x)

$$a(x, t)u_t + b(x, t)u_x + c(x, t)u = f(x, t) \quad (1.2)$$

2. Quasilinear¹ first order PDE (the equation is only linear in u_t, u_x)

$$a(x, t, u)u_t + b(x, t, u)u_x = f(x, t, u) \quad (1.3)$$

The initial condition $u(x, 0)$ is specified at $t = 0$

$$u(x, 0) = f(x) \quad (1.4)$$

¹Such quasilinear equations are solved using the Method of Characteristics

1.2 Euler's Equations of Gas Dynamics

At the very core we are interested in physical quantities like Density (ρ), Velocity (u), Pressure (p) represented in a vector of **Primitive Variables**.

$$V = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} \rho \\ u \\ p \end{pmatrix} \quad (1.5)$$

but it is difficult to work with these variables in conditions important to us which involve **discontinuities** like *shock-waves*. So, we transform these variables into those which arise more naturally in conservation systems like Density (ρ), Momentum (ρu) and Total Energy (E) per unit mass represented in a vector of **Conserved Variables**.

$$U = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} \quad (1.6)$$

In physics, these conserved variables result naturally from the application of fundamental laws like

1. Conservation of Mass (*Continuity Equation*)
2. Newton's Second Law (*Momentum Equation*)
3. Laws of Conservation of Energy (*Energy Equation*)

and numerical computation is easier for those physical laws when they are expressed in terms of Conserved Variables.

We work first under the assumption that these conserved quantities are sufficiently smooth to allow for the operation of differentiation to be defined. However, later this assumption is removed to allow for solutions containing discontinuities like shock waves.

The hyperbolic system of conservation laws which we are concerned with read as

$$U_t + F(U)_x = 0 \quad (1.7)$$

where x is a spatial variable, t is time, $U(x, t) \in \mathbb{R}^N$, and F is a flux vector. This system can be expanded and written as follows

$$\rho_t + (\rho u)_x = 0 \quad (1.8)$$

$$(\rho u)_t + (\rho u^2 + p)_x = 0 \quad (1.9)$$

$$E_t + [u(E + p)]_x = 0 \quad (1.10)$$

1.3 Classifying Euler's equations

In order to develop solutions for the Euler's system, we first need to understand in what categories to classify it. To successfully classify the equations we first observe the compact vector form of the equation

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0 \quad (1.11)$$

We should convert this system to its **Quasi Linear Form** using chain rule in order to understand it better

$$F(U)_x = \left(\frac{dF}{dU}\right) \frac{\partial U}{\partial x} \quad (1.12)$$

$$\frac{\partial U}{\partial t} + \left(\frac{dF}{dU}\right) \frac{\partial U}{\partial x} = 0 \quad (1.13)$$

Here, $\frac{dF}{dU}$ is a 3×3 matrix called the **Flux Jacobian** and is of the form

$$\frac{dF}{dU} = \begin{pmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} & \frac{\partial f_1}{\partial u_3} \\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2} & \frac{\partial f_2}{\partial u_3} \\ \frac{\partial f_3}{\partial u_1} & \frac{\partial f_3}{\partial u_2} & \frac{\partial f_3}{\partial u_3} \end{pmatrix} \quad (1.14)$$

Now to find the entries of the matrix, we need to express² all the f_i in terms of u_i in order to perform the differentiations. We have,

$$F(U) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u(E + p) \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \end{pmatrix} \quad (1.16)$$

We convert every element one by one as follows

$$f_1 = \rho u = u_2 \quad (1.17)$$

$$f_2 = \rho u^2 + p = (\gamma - 1)u_3 + \left(\frac{3 - \gamma}{2}\right) \frac{u_2^2}{u_1} \quad (1.18)$$

$$f_3 = u(E + p) = \frac{u_2 u_3}{u_1} \gamma - (\gamma - 1) \frac{u_2^3}{2u_1^2} \quad (1.19)$$

²We also need the very useful **Equation of State** which is

$$E = \frac{p}{\gamma - 1} + \frac{\rho u^2}{2} \quad (1.15)$$

Thus we have the required **Flux Jacobian**

$$\frac{dF}{dU} = \begin{pmatrix} 0 & 1 & 0 \\ -\frac{u_2^2}{u_1^2}(\frac{3-\gamma}{2}) & \frac{u_2}{u_1}(3-\gamma) & \gamma-1 \\ -\frac{u_2 u_3}{u_1^2}\gamma + (\gamma-1)\frac{u_2^3}{u_1^3} & \frac{u_3}{u_1}\gamma - \frac{3}{2}(\gamma-1)\frac{u_2^2}{u_1^2} & \frac{u_2}{u_1}\gamma \end{pmatrix} \quad (1.20)$$

Note³ that,

$$H = \frac{E+p}{\rho} \quad (1.21)$$

$$a^2 = \frac{\gamma p}{\rho} \quad (1.22)$$

Ultimately we have the relation,

$$H = \frac{a^2}{\gamma-1} + \frac{u^2}{2} = \frac{u_3}{u_1}\gamma - \frac{u_2^2}{u_1^2}(\frac{\gamma-1}{2}) \quad (1.23)$$

which we use in the Flux jacobian matrix in the terms $\frac{\partial f_3}{\partial u_1}$ and $\frac{\partial f_3}{\partial u_2}$ to get

$$\frac{dF}{dU} = \begin{pmatrix} 0 & 1 & 0 \\ (\frac{\gamma-3}{2})u^2 & (3-\gamma)u & \gamma-1 \\ u[(\frac{\gamma-1}{2})u^2 - H] & H - (\gamma-1)u^2 & \gamma u \end{pmatrix} \quad (1.24)$$

This is the required form of the Flux Jacobian which is used to calculate the eigenvalues and eigenvectors of the matrix which are as follows

$$\lambda = u - a, u, u + a \quad (1.25)$$

and corresponding eigenvectors are

$$\begin{pmatrix} 1 \\ u - a \\ H - ua \end{pmatrix}, \begin{pmatrix} 1 \\ u \\ \frac{u^2}{2} \end{pmatrix}, \begin{pmatrix} 1 \\ u + a \\ H + ua \end{pmatrix} \quad (1.26)$$

Observe the three eigenvectors are **linearly independent**, hence the Euler's Equation's of Gas Dynamics form a **Hyperbolic System of Conservation Laws**.

As a rule of thumb, whenever information travells at **finite speed**, it is modelled using a Hyperbolic system of PDE's.

³ a is the **speed of sound** here

1.4 Summary

Summary of various forms of Euler Equations of Gas Dynamics.

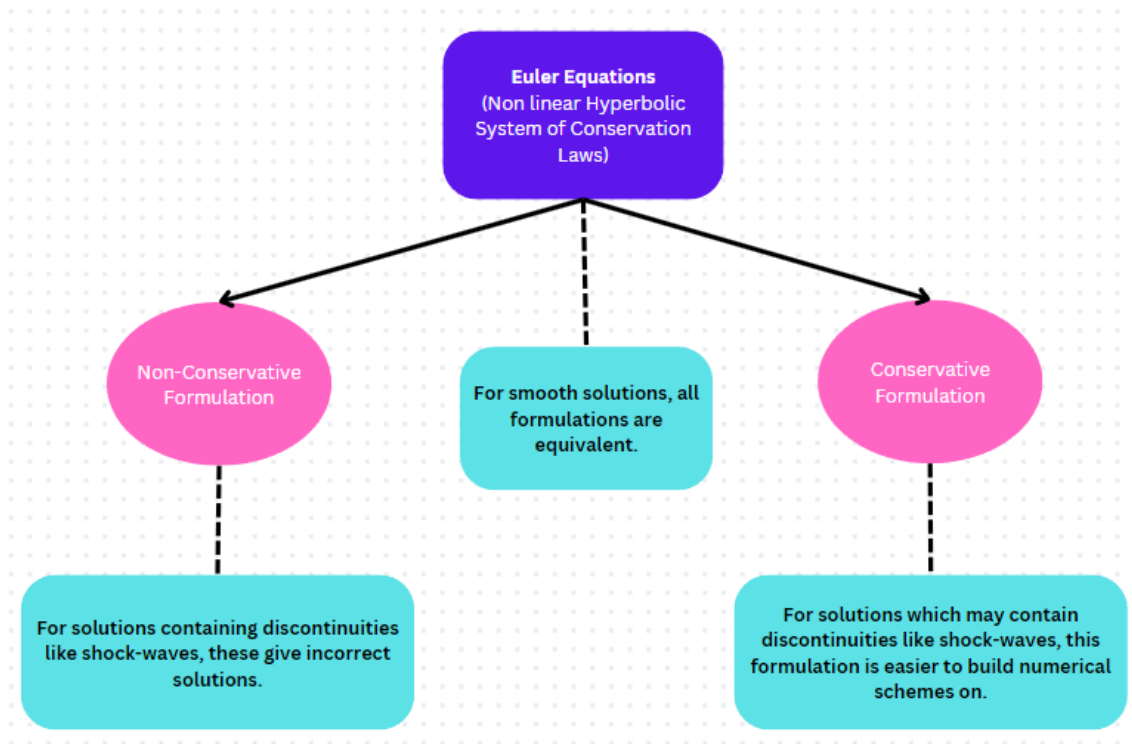


Figure 1.1: Different forms of Euler's Equations

Chapter 2

Numerical Schemes

2.1 Second-order semi-discrete central-upwind (CU) scheme

Here, a brief description of the second-order semi-discrete CU schemes for the Euler's system from [2] is provided.

2.1.1 One-dimensional CU Scheme

We split the computational domain into **the finite-volume** cells $C_j := [x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$, which for the sake of brevity are assumed to be uniform. As in all finite-volume methods, the computed solution is realized in terms of its cell averages.

$$\bar{U}_j(t) \approx \frac{1}{\Delta x} \int_{C_j} U(x, t) dx \quad (2.1)$$

They are assumed to be known at a given time t , and are then evolved in time according to the following semi-discretization:

$$\frac{d}{dt} \bar{U}_j = - \frac{\mathbb{F}_{j+\frac{1}{2}} - \mathbb{F}_{j-\frac{1}{2}}}{\Delta x} \quad (2.2)$$

This is the general framework for Finite Volume Schemes and the quality of a scheme lies in selection of the Numerical Flux $\mathbb{F}_{j+\frac{1}{2}}$.

The CU numerical flux which was originally derived in [3, 4] and later modified in [2] which is defined as:

$$\mathbb{F}_{j+\frac{1}{2}} = \frac{a_{j+\frac{1}{2}}^+ F(U_j^E) - a_{j+\frac{1}{2}}^- F(U_{j+1}^W)}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-} + \frac{a_{j+\frac{1}{2}}^+ a_{j+\frac{1}{2}}^-}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-} [U_{j+1}^W - U_j^E - \delta U_{j+\frac{1}{2}}] \quad (2.3)$$

Calculating the CU Numerical Flux

Let's look at the steps required for the calculation of this flux one by one.

First we calculate the slopes $(U_x)_j$ which are used later in calculation of the respective point values of the **Piecewise Linear Reconstruction**, i.e., U_j^E and U_{j+1}^W .

$$U_j^E = \bar{U}_j + \frac{\Delta x}{2} (U_x)_j, \quad U_{j+1}^W = \bar{U}_j - \frac{\Delta x}{2} (U_x)_j \quad (2.4)$$

Where,

$$(U_x)_j = \text{minmod}\left(\theta \frac{\bar{U}_j - \bar{U}_{j-1}}{\Delta x}, \frac{\bar{U}_{j+1} - \bar{U}_{j-1}}{2\Delta x}, \theta \frac{\bar{U}_{j+1} - \bar{U}_j}{\Delta x}\right) \quad (2.5)$$

Here, $\theta \in [1, 2]$ is a tuning parameter which helps to control the sharpness of resulting reconstructions and the minmod function is defined as,

$$\text{minmod}(z_1, z_2, \dots) := \begin{cases} \min\{z_k\}, & \text{if } z_k > 0 \forall k, \\ \max\{z_k\}, & \text{if } z_k < 0 \forall k, \\ 0, & \text{otherwise} \end{cases} \quad (2.6)$$

After calculating the Piecewise Linear Reconstruction, we now calculate the **one-sided local speeds of propagation**¹ which are estimated as follows

$$a_{j+\frac{1}{2}}^+ = \max\{\lambda_N\left(\frac{\partial F}{\partial U}(U_{j+1}^W)\right), \lambda_N\left(\frac{\partial F}{\partial U}(U_j^E)\right), 0\} \quad (2.7)$$

$$a_{j+\frac{1}{2}}^- = \min\{\lambda_1\left(\frac{\partial F}{\partial U}(U_{j+1}^W)\right), \lambda_1\left(\frac{\partial F}{\partial U}(U_j^E)\right), 0\} \quad (2.8)$$

Where, $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_N$ are the N eigenvalues of the **flux jacobian** $\frac{\partial F}{\partial U}$. The built-in **anti-diffusion** term $\delta U_{j+\frac{1}{2}}$ is given by

$$\delta U_{j+\frac{1}{2}} = \text{minmod}(U_{j+1}^W - U_{j+\frac{1}{2}}^*, U_{j+\frac{1}{2}}^* - U_{j+1}^W) \quad (2.9)$$

where

$$U_{j+\frac{1}{2}}^* = \frac{a_{j+\frac{1}{2}}^+ U_{j+1}^W - a_{j+\frac{1}{2}}^- U_j^E - \{F(U_{j+1}^W) - F(U_j^E)\}}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-} \quad (2.10)$$

¹The way these local speeds of propagation are approximated also affects the quality of the solution as done in [1]

Thus, given the cell averages \bar{U}_j at some time $t = t_0$, we can find the CU Numerical Flux $\mathbb{F}_{j+\frac{1}{2}}$.

Time Discretization

Let us consider 2.2 again

$$\frac{d}{dt}\bar{U}_j = -\frac{\mathbb{F}_{j+\frac{1}{2}} - \mathbb{F}_{j-\frac{1}{2}}}{\Delta x} \quad (2.11)$$

We can use the simple **Euler Forward Difference** in LHS for time discretization, but for more accuracy we use the **Three Stage - Strong Stability Preserving Runge-Kutta(SSP-RK)** time discretization which is as follows,

$$U^1 = U^n + \Delta t R(U^n) \quad (2.12)$$

$$U^2 = \frac{3}{4}U^n + \frac{1}{4}U^1 + \frac{1}{4}\Delta t R(U^1) \quad (2.13)$$

$$U^{n+1} = \frac{1}{3}U^n + \frac{2}{3}U^2 + \frac{2}{3}\Delta t R(U^2) \quad (2.14)$$

Where,

$$\frac{dU_j}{dt} = -\frac{1}{\Delta x}[F_{j+\frac{1}{2}}^n - F_{j-\frac{1}{2}}^n] = R(U) \quad (2.15)$$

And U^n is the solution which we have at t , using which we calculate U^1 and U^2 . Then U^{n+1} is the solution at the next time step $t + \Delta t$.

CFL

The Courant-Friedrichs-Lewy (CFL) Condition is a condition for stability for numerical methods that model convection or wave phenomena. In our one dimensional case, the maximum speed of information transfer is λ_N , i.e., $|u| + a$. If the volume of a finite volume cell is Δx , then for stability we have

$$(|u| + a) \times \Delta t \leq \Delta x \quad (2.16)$$

$$\implies \Delta t = \frac{\epsilon \Delta x}{\max(|u| + a)} \quad (2.17)$$

Usually, the constant $\epsilon = \text{CFL} = 0.45$.

2.1.2 Two-dimensional CU Scheme

The CU Scheme used for one-dimensions can be extended to two-dimensions using dimensional splitting.

Chapter 3

CU Scheme on Riemann Problem

3.1 The Riemann Problem

The Riemann problem is the simplest non-trivial Initial Value Problem(IVP) for Euler's System in 1D. The problem read's as follows

$$U(x, 0) = U^{(0)}(x) = \begin{cases} U_L, & \text{if } x < 0 \\ U_R, & \text{if } x > 0 \end{cases} \quad (3.1)$$

3.1.1 Results of CU Scheme on various problems

Now we show some of the results recreated as a part of this initial Literature Review for the Bathchelor's Thesis Project.

Moving Contact Wave

We consider the initial conditions

$$(\rho(x, 0), u(x, 0), p(x, 0)) = \begin{cases} (1.4, 0.1, 1), & x < 0.3 \\ (1.0, 0.1, 1), & x > 0.3 \end{cases} \quad (3.2)$$

Where the computational domain is $x \in [0, 1]$ and solution is evolved till $t = 2\text{sec}$ on a uniform grid, for a second-order scheme we take $\Delta x = \frac{1}{200}$. Free boundary conditions are imposed. Results are summarised in figure 3.1, along with initial conditons, solution evolved by CU scheme and a reference plot¹.

¹Reference plots are generated using the same scheme but with a finer finite volume mesh, usually 4 times finer than the solution

Lax Problem

We consider the initial conditions

$$(\rho(x, 0), u(x, 0), p(x, 0)) = \begin{cases} (0.445, 0.698, 3.528), & x < 0 \\ (0.500, 0.000, 0.571), & x > 0 \end{cases} \quad (3.3)$$

Where the computational domain is $x \in [-5, 5]$ and solution is evolved till $t = 1.3\text{sec}$ on a uniform grid, for a second-order scheme we take $\Delta x = \frac{1}{200}$. Free boundary conditions are imposed. Results are summarised in figure 3.2.

Sod's shock tube problem

We consider the initial conditions

$$(\rho(x, 0), u(x, 0), p(x, 0)) = \begin{cases} (1.0, 0, 100000), & x < 0 \\ (0.125, 0, 10000), & x > 0 \end{cases} \quad (3.4)$$

Where the computational domain is $x \in [-10, 10]$ and solution is evolved till $t = 0.01\text{sec}$ on a uniform grid, for a second-order scheme we take $\Delta x = \frac{1}{200}$. Free boundary conditions are imposed. Results are summarised in figure 3.3.

Blastwave Problem

We consider the initial conditions

$$(\rho(x, 0), u(x, 0), p(x, 0)) = \begin{cases} (1, 0, 1000), & x < 0.1 \\ (1, 0, 0.01), & 0.1 \leq x \leq 0.9 \\ (1, 0, 100), & x > 0.9 \end{cases} \quad (3.5)$$

Where the computational domain is $x \in [0, 1]$ and solution is evolved till $t = 0.038\text{sec}$ on a uniform grid, for a second-order scheme we take $\Delta x = \frac{1}{400}$. Reflective boundary conditions are imposed. Results are summarised in figure 3.4. This is the ultimate problem in one-dimension and is a prototype to modelling the effects of Nuclear Weapons in three-dimensions.

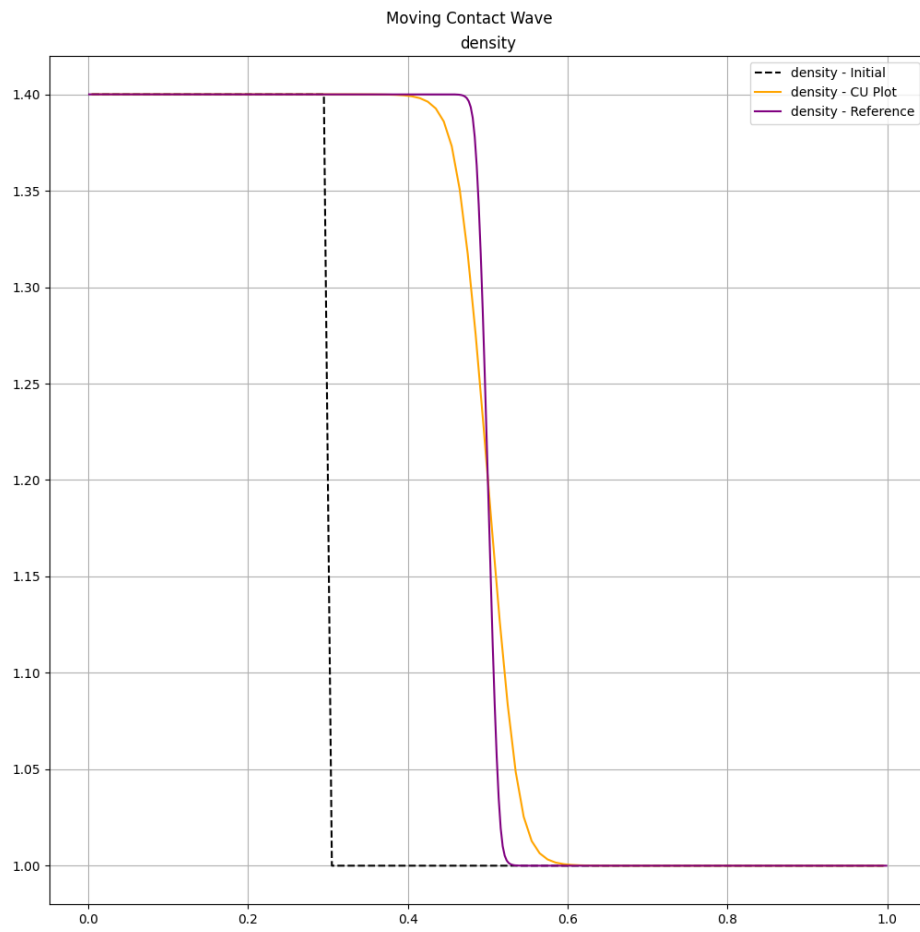


Figure 3.1: Moving Contact Wave

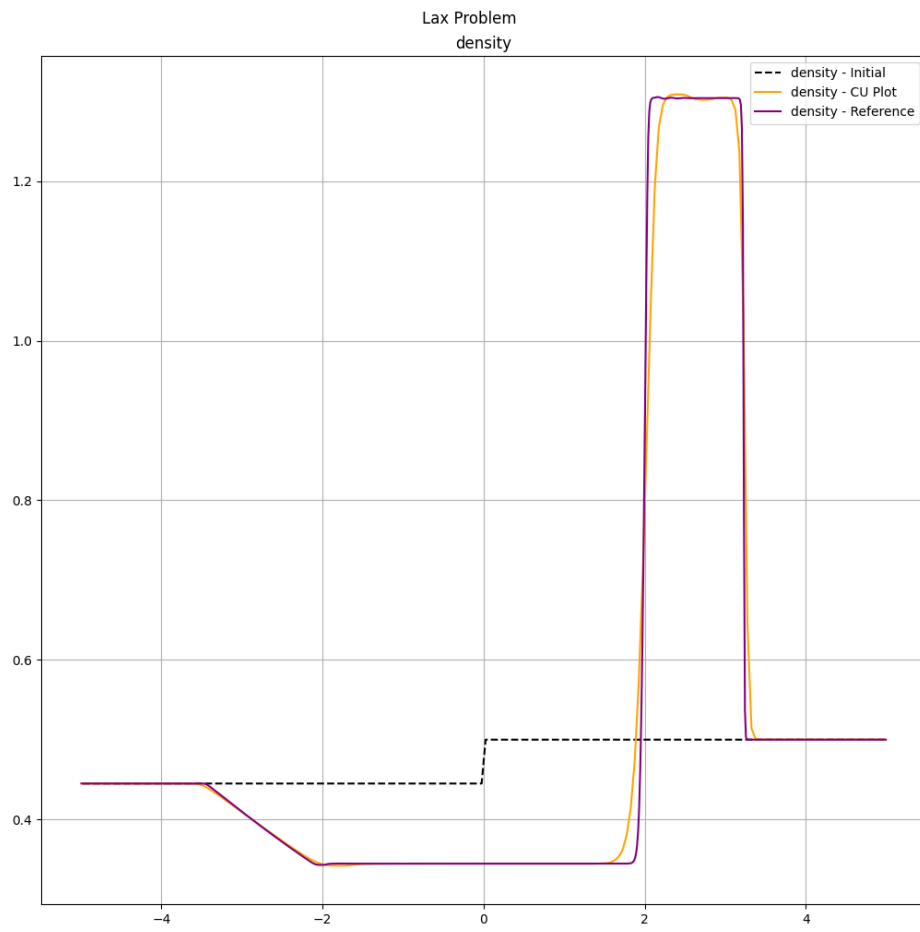


Figure 3.2: Lax problem

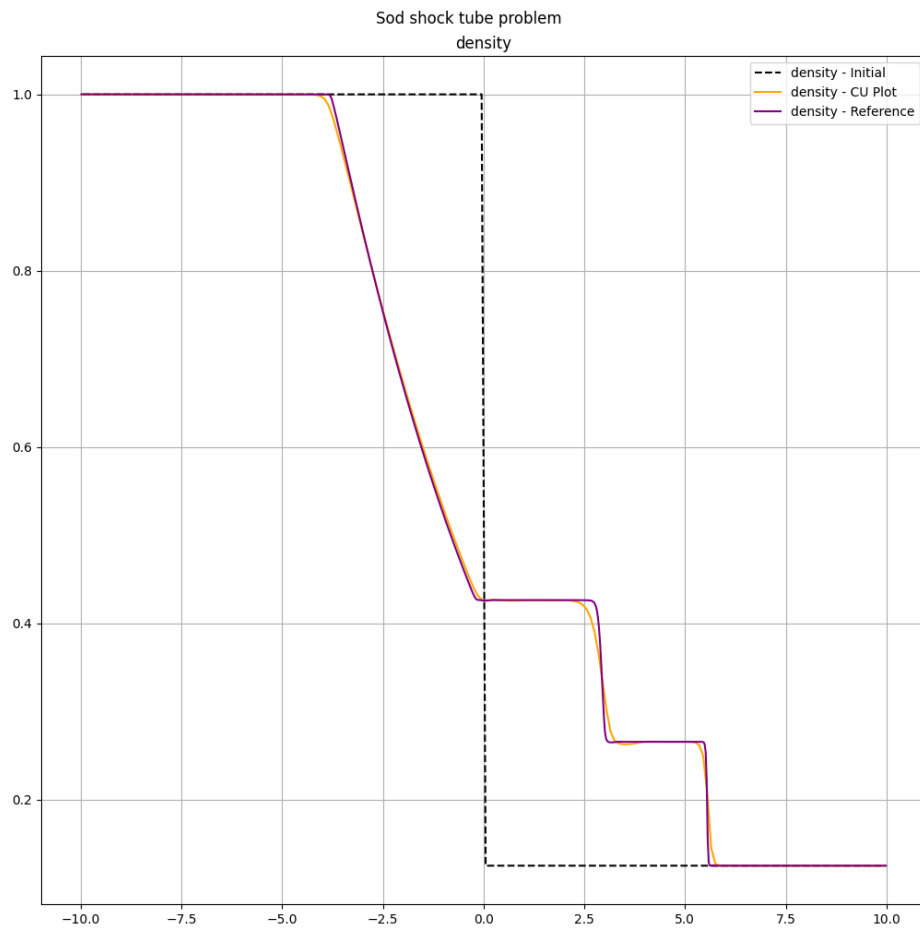


Figure 3.3: Sod's Shock Tube Problem

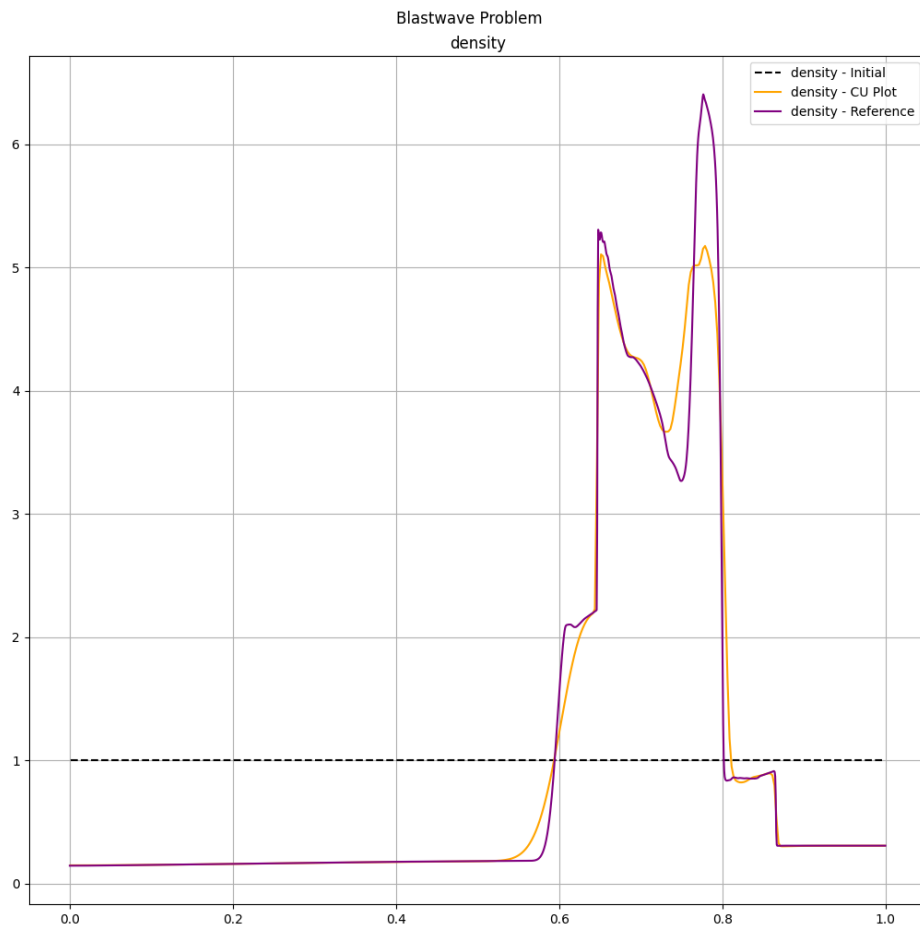


Figure 3.4: Blast Wave Problem

Chapter 4

Future work

The present study has provided an initial understanding of numerical schemes for the time-dependent compressible Euler equations of gas dynamics, primarily focusing on foundational theories of nonlinear hyperbolic systems of partial differential equations (PDEs) and exploring the renowned Central Upwind (CU) scheme in one dimension. However, several avenues for further exploration and refinement exist, paving the way for future research and development in this field.

Exploration of the Two-Dimensional CU Scheme

An immediate objective in the upcoming phase of this project involves a comprehensive study of the two-dimensional Central Upwind scheme. Extending the current knowledge from the one-dimensional domain to higher dimensions using dimensional splitting. Exploring its application in two dimensions will necessitate an in-depth analysis of the computational complexities, stability, and accuracy of the scheme in a multi-dimensional space.

Detailed Theoretical Investigation

Further advancement will focus on a more detailed theoretical analysis for the numerical schemes in both one and two dimensions. This will involve a rigorous study of the underlying mathematical principles, stability analysis, and the derivation of convergence properties, shedding light on the scheme's robustness under various conditions.

Applying High Performance Parallel Computing

The studied scheme is highly parallelizable in nature and an exploration for the performance gains using this will be explored in the future.

Extended Research in Related Fields

Expanding the scope of research will involve delving deeper into related fields that intersect with numerical schemes for hyperbolic PDEs. This includes but is not limited to exploring other numerical methods for solving compressible Euler equations, investigating different discretization techniques, and comparing their performance and limitations in various scenarios.

The roadmap outlined here forms the basis for the next phase of this research. By embarking on these future tasks, it is anticipated that a more comprehensive understanding of numerical schemes for time-dependent compressible Euler equations will be achieved, laying the groundwork for potential advancements in this domain.

Chapter 5

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