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Thermodynamically Compatible Finite Volume Schemes

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Contents

1 Introduction

A family of semidiscrete and fully discrete finite volume schemes for overdetermined, hyperbolic and thermodynamically compatible PDE systems in various dimensions are studied. In particular, we consider the Euler equations of the magnetodynamics (MHD) , with suitable relaxation of some source terms. In 1961, Godunov published his groundbreaking paper "An interesting class of quasilinear systems" , in which he discovered the connection between symmetric hyperbolicity in the sense of Friedrichs and thermodynamic compatibility (SHTC), ten years before Friedrichs and Lax , who independently rediscovered the same connection again in 1971. In a subsequent series of papers, Godunov and Romenski carried out further research on this link between symmetric hyperbolicity and thermodynamic compatibility and generalized the seminal idea of Godunov to the more general SHTC framework of symmetric hyperbolic and thermodynamically compatible systems, which includes not only the compressible Euler equations of gasdynamics, but also the magnetohydrodynamics (MHD) equations and the equations of nonlinear hyperelasticity. The main aim is to mimic the SHTC (symmetric hyperbolic thermodynamic compatible) framework also on the discrete level by directly discretizing the entropy inequality, instead of the total energy conservation law, while the total energy conservation is obtained via an appropriate linear combination as a consequence of the thermodynamically compatible discretization of all equations.

SHTC systems can go beyond classical mechanics. Despite the mathematical beauty and rigor of the SHTC framework, upto now it has not been carried much over to the discrete level.

2 Turbulent Shallow Water Flow Systems

The mathematical model of shear shallow water flows of constant density is studied. A novel reformulation based on a decomposition of the Reynolds stress tensor $\mathbf{P}$ as $\mathbf{P} = \mathbf{Q}\mathbf{Q}^{\mathbf{T}}$. Further, viscous terms are introduced ad finally, we prove that the proposed viscous system is thermodynamically compatible with energy conservation and entropy inequality.

2.1 Governing Equations

Considering the over-determined hyperbolic model for turbulent shear shallow water flows in multiple space dimensions in gravity free space and non-viscous system (i.e. $g = 0, b = 0, and, C_f = 0$), we have

$$\boxed{\partial_t h + \nabla \cdot (h\mathbf{v}) = 0} \tag{1}$$

$$\boxed{\partial_t (h\mathbf{v}) + \nabla \cdot (h\mathbf{v} \otimes \mathbf{v} + h\mathbf{P}) = 0} \tag{2}$$

$$\boxed{\partial_t \mathbf{P} + v \cdot \nabla \mathbf{P} + \nabla \mathbf{v} \mathbf{P} + \mathbf{P} \nabla \mathbf{v}^{\mathbf{T}} = 0} \tag{3}$$

So, through energy conservation law, we get the following equations:

$$\partial_t (hE) + \nabla \cdot (\mathbf{v}(hE) + hP\mathbf{v}) = 0 \tag{4}$$

Also, the total energy is defined as:

$$hE = \frac{1}{2} h||\mathbf{v}|| + \frac{1}{2} h\mathbf{P} \tag{5}$$

2.2 Reformulaton of the Model

For hyperbolicity, this model requires $tr\mathbf{P} \geq 0$.
In order to gaurantee this property also at the discrete level for all times, we will have refomulation of the system (1)-(3). We will first look at the following homogeneous equation for the symmetric tensor $\mathbf{P}$:

$$\dot{\mathbf{P}} + \mathbf{L}\mathbf{P} + \mathbf{P}\mathbf{L}^{\mathbf{T}} = 0 \tag{6}$$

Here, for any f, $\dot{f}$ means the material time derivative: $\dot{f} = f_t + \mathbf{v} \cdot \nabla$

$$\mathbf{L} = \frac{\partial \mathbf{v}}{\partial \mathbf{x}} = \nabla \mathbf{v}. \tag{7}$$

Let us replace $\mathbf{P}$ by $\mathbf{P} = \mathbf{Q}\dot{\mathbf{Q}}$
Thus, the transformed equations with $\mathbf{P}$ replaced by $\mathbf{P} = \mathbf{Q}\dot{\mathbf{Q}}$ will be as follows:

$$(\dot{\mathbf{Q}} + \mathbf{L}\mathbf{Q})\mathbf{Q}^{\mathbf{T}} + \mathbf{Q}(\dot{\mathbf{Q}} + \mathbf{L}\mathbf{Q}) = 0 \tag{8}$$

If $\dot{\mathbf{Q}} + \mathbf{L}\mathbf{Q} = \mathbf{B}(\mathbf{Q}^{\mathbf{T}})^{\mathbf{-1}}$, with an antisymmetric tensor $\mathbf{B} = -\mathbf{B}^{\mathbf{T}}$, we can observe that the equations for $\mathbf{P}$ will be satisfied automatically.

2.3 What is the geometrical sense of decomposition $\mathbf{P} = \mathbf{Q}\mathbf{Q}^{\mathbf{T}}$?

Gram matrix with two vectors $\mathbf{w_i}$, $i = 1, 2$ is as follows:

$$\mathbf{G} = \begin{pmatrix} \mathbf{w_1} \cdot \mathbf{w_1} & \mathbf{w_1} \cdot \mathbf{w_2} \\ \mathbf{w_1} \cdot \mathbf{w_2} & \mathbf{w_2} \cdot \mathbf{w_2} \end{pmatrix} \tag{9}$$

Here, the dot defines the scalar product of vectors. So, it can be written as:

$$\mathbf{G} = \mathbf{Q}\mathbf{Q}^{\mathbf{T}} \tag{10}$$

We can see that in our case $\mathbf{P}$ is the correlation tensor, expressed in terms of the velocity pulsations, as follows:

$$\mathbf{P} = \begin{pmatrix} \overline{v_1'^2} & \overline{v_1' v_2'} \\ \overline{v_1' v_2'} & \overline{v_2'^2} \end{pmatrix} \tag{11}$$

Here, the averaging is the depth averaging, which is denoted by a "bar".
Claim: $\mathbf{P}$ can be presented in the form of (9), i.e., we can have vectors $\mathbf{w_i}$ such that:

$$\mathbf{P} = \begin{pmatrix} \mathbf{w_1} \cdot \mathbf{w_1} & \mathbf{w_1} \cdot \mathbf{w_2} \\ \mathbf{w_1} \cdot \mathbf{w_2} & \mathbf{w_2} \cdot \mathbf{w_2} \end{pmatrix}$$

Clearly, we take $\mathbf{w_1} = \sqrt{\overline{v_1'^2}}(Cos\theta_1, Sin\theta_1)^{\mathbf{T}}, \mathbf{w_2} = \sqrt{\overline{v_2'^2}}(Cos\theta_2, Sin\theta_2)^{\mathbf{T}}$ with $Cos(\theta_1 - \theta_2) = \frac{\overline{\mathbf{v_1' v_2'}}}{\sqrt{\overline{\mathbf{v_1'^2 v_2'^2}}}}$ for this and this satisfies our claim. The last relation is well defined because of Cauchy-Schwartz inequality.
Now, with $P_{ik} = Q_{im}Q_{km}$, the equations (1)-(3) is modified as follows:

$$\partial_t h + \partial_m (h v_m) = 0 \tag{12}$$

$$\partial_t(hv_i) + \partial_k(hv_iv_k + hP_{ik}) = 0 \tag{13}$$

$$\partial_t Q_{ik} + v_m\partial_m Q_{ik} + (\partial_m v_i)Q_{mk} = 0 \tag{14}$$

It can be seen that this new system has an extra energy conservation law, which can be obtainded from (12) - (14)

$$\partial_t(hE) + \partial_i((hE)v_i + hQ_{im}Q_{km}v_k) = 0 \tag{15}$$

The time derivative of the determinant of $\mathbf{Q}$ can be obtained via the Jacobi formula, using which we can express the derivative of the determinant of a matrix in terms of the inverse of the matrix and the derivatives of the matrix itself:

$$\partial_t|Q| = |Q|Q^{-1}_{ki}\partial_t Q_{ik}, \quad \partial_m|Q| = |Q|Q^{-1}_{ki}\partial_m Q_{ik} \tag{16}$$

where Q^{-1}_{ki} is a compact notation for $(Q^{-1})_{ki}$. Using (16) in (14), we get

$$\partial_t|Q| + |Q|Q^{-1}_{ki}v_m\partial_m Q_{ik} + |Q|Q^{-1}_{ki}(\partial_m v_i)Q_{mk} = 0 \tag{17}$$

$$\implies \partial_t|Q| + v_m\partial_m|Q| + |Q|(\partial_m v_i)\partial_{mi} = 0 \tag{18}$$

$$\implies \partial_t|Q| + \partial_m(v_m|Q|) = 0 \tag{19}$$

The equation (20) is same as he mass conservation equation (12);

$$Taking \quad \psi = \frac{|\mathbf{P}|}{h^2} = \frac{|\mathbf{Q}\mathbf{Q}^\mathbf{T}|}{h^2}, \quad \partial_t(h\psi) + \partial_m(v_m h\psi) = 0 \tag{20}$$

2.4 Godunov Form of Nonlinear Systems of Hyperbolic Conservation laws

Firstly, we consider only hyperbolic systems of conservation laws in two space dimensions of the type:

$$\mathbf{q_t} + \partial_k \mathbf{f_k} = 0 \tag{21}$$

along with flux tensor $\mathbf{F} = \mathbf{(f_1, f_2)}$, and after the parametrization according to the Godunov, we get

$$(L_p)_t + \partial_k((v_k L)_p) = 0 \tag{22}$$

along with the conservation law of the form:

$$\mathcal{E}_t + \partial_k \mathbf{F_k} = 0 \tag{23}$$

where $\mathbf{F_k}$ is the total energy flux in the k-th coordinate direction. Equation (22)-(23) are called *Godunov form of conservation law* and gives an overdetermined system of PDE. This system is thermodynamically compatible if the following conditions hold:

$$\mathbf{q} = L_p, \quad \mathbf{p} = \mathcal{E}_q, \quad \mathbf{f}_k = (v_k L)_p, \quad F_k = \mathbf{p}\cdot\mathbf{f}_k - v_k L \tag{24}$$

Here, L is called *generating potential* and $\mathcal{E}$ is the total energy density, which are Legendre transform of each other and thus satisfy the following criteria:

$$L = \mathbf{p}\cdot\mathbf{q} - \mathcal{E}, \quad \mathcal{E} = \mathbf{p}\cdot\mathbf{q} - L \tag{25}$$

L and $\mathcal{E}$ are assumed to be strictly convex functions of their arguments, and thus the transformation matrices between $\mathbf{p}$ and $\mathbf{q}$, which are Hessian matrices of L and $\mathcal{E}$, respectively satisfy:

$$\frac{\partial \mathbf{p}}{\partial \mathbf{q}} = \mathcal{E}_{qq} > 0, \quad \frac{\partial \mathbf{q}}{\partial \mathbf{p}} = L_{pp} > 0, \quad L_{pp} = (\mathcal{E}_{qq})^{-1} \tag{26}$$

$$L_{pp} = L^T_{\mathbf{pp}}, \quad \mathcal{E}_{qq} = \mathcal{E}^T_{\mathbf{qq}} \tag{27}$$

Claim: Equation (23) is a consequence of Equation(22).

$$\begin{aligned}
&(L_p)_t + \partial_k((v_k L)_p) = 0 \\
\implies &\mathbf{p}\cdot(\mathbf{L_p})_\mathbf{t} + \mathbf{p}\cdot\partial_k\mathbf{f}_k = 0 \\
\implies &(\mathbf{p}L_p)_t - \mathbf{p}_t L_p + \partial_k(\mathbf{p}\cdot\mathbf{f}_k) - (\partial_k\mathbf{p})\cdot\mathbf{f_k} = 0 \\
\implies &\frac{\partial}{\partial_t}(\mathbf{p}L_p) - L_t + \partial_k(\mathbf{p}\cdot\mathbf{f}_k) - \partial_k\mathbf{p}\cdot(v_k L)_p = 0 \\
\implies &\frac{\partial}{\partial_p}(\mathbf{p}L_p)\mathbf{p}_t - L_t + \partial_k F_k = 0 \\
\implies &(\mathbf{p}L_{pp} + L_p)\mathbf{p}_t - L_t + \partial_k F_k = 0 \\
\implies &\left(\mathbf{p}\frac{\partial\mathbf{q}}{\partial\mathbf{p}} + \mathbf{q}\right)\mathbf{p}_t - L_t + \partial_k F_k = 0 \\
\implies &\left(\frac{\partial}{\partial\mathbf{p}}(\mathbf{p}\cdot\mathbf{q})\right)\mathbf{p}_t - L_t + \partial_k F_k = 0 \\
\implies &\left(\frac{\partial}{\partial\mathbf{p}}(\mathbf{p}\cdot\mathbf{q})\right)\mathbf{p}_t - L_t + \partial_k F_k = 0 \\
\implies &\frac{\partial}{\partial p}(\mathcal{E} + L) - L_t + \partial_k F_k = 0 \\
\implies &\mathcal{E}_t + \partial_k F_k = 0
\end{aligned} \tag{28}$$

Equivalently, the shallow water subsystem for flat bottom is as follows:

$$\partial_t h + \partial_k(h v_k) = 0 \tag{29}$$

$$\partial_t(h v_i) + \partial_k(h v_i v_k) = 0 \tag{30}$$

$$\partial_t\mathcal{E} + \partial_k(\mathcal{E} v_k) = 0 \tag{31}$$

2.5 Thermodynamically Compatible vanishing Viscosity Limit

Here, we will assume flat bottom, b = 0, along with $\alpha = C_f = 0$, but in order to guarantee the exact total energy conservation, a non negative term T_{ik} is added to the governing PDE for $\mathbf{Q}$:

$$\partial_t h + \partial_m(h v_m) = \partial_m\epsilon\partial_m h \tag{32}$$

$$\partial_t(h v_i) + \partial_k(h v_i v_k + h P_{ik}) = \partial_m\epsilon\partial_m(h v_i) \tag{33}$$

$$\partial_t Q_{ik} + v_m\partial_m Q_{ik} + (\partial_m v_i)Q_{mk} = \partial_m\epsilon\partial_m Q_{ik} + T_{ik} \tag{34}$$

$$\partial_t\mathcal{E} + \partial_i((\mathcal{E}_1 + \mathcal{E}_2)v_i + (h P_{ik})v_k) = \partial_m\epsilon\partial_m\mathcal{E} \tag{35}$$

where, $\epsilon > 0$ is the dissipation coefficient, associated with the small parabolic dissipation term, is added to the equations.
Now, the total energy $\mathcal{E} = hE = \mathcal{E}_1 + \mathcal{E}_2$ can be divided into $\mathcal{E}_1 = hE_1 = \frac{1}{2}h v_i v_i$ and $\mathcal{E}_2 = hE_2 = \frac{1}{2}h Q_{ik}Q_{ik}$, and thus $\mathcal{E}_1$ is the total potential energy associated with the shallow water subsystem (31)-(34), while $\mathcal{E}_2$ is the total energy associated with the object Q_{ik}.
Further, we will now denote the inviscid part of the total energy flux through the following equation:

$$\mathbf{F} = (\mathcal{E}_1 + \mathcal{E}_2)v_i + h P_{ik}v_k = \mathbf{F_G} + \mathcal{E}_2 v_i + h P_{ik}v_k \tag{36}$$

where,

$$\mathbf{F_G} = \mathcal{E}_1 v_i \tag{37}$$

whose usuage we will see later on.
The production term, T_{ik}, which is needed for the consistency of the total energy conservation, is formulated as follows:

$$T_{ik} = \epsilon \frac{Q_{ik}}{htr\mathbf{P}} \partial_m q_i (\mathcal{E}_{q_i q_j}) \partial_m q_j \tag{38}$$

Theorem 1. *(Energy Conservation) The energy conservation law (34) is a consequence of the equations (31) - (33).*

Proof. The black terms in the equations (31) - (32) can be directly deduced from the general class of PDE (22) - (23) by Godunov. So, the compatibilty of the shallow water system with the energy conservation law with energy potential $\mathcal{E}$ is trivial. So, now, we have to consider only the remaining terms associated with the quantity Q_{ik}, which are coloured with red, and the viscous terms, which are coloured in blue.
Now, we will show the compatibility of the red terms. Since, $(\mathcal{E}_2)_h = E_2 = \frac{1}{2} Q_{ik} Q_{ik} = \frac{1}{2} tr\mathbf{P}, \mathcal{E}_{hv_i} = v_i, \mathcal{E}_{Q_{ik}} = (\mathcal{E}_2)_{Q_{ik}} = h(E_2)_{Q_{ik}} = hQ_{ik}$, now the summation of (31) - (33) with the thermodynamic dual variables and considering only the new contributions that are not yet contained in the Godunov-form □

Theorem 2. *(Entropy-type Inequality) A direct consequence of the PDE (34) without the parabolic dissipative term, i.e., of the equation*

$$\partial_t Q_{ik} + v_m \partial_m Q_{ik} + (\partial_m v_i) Q_{mk} = T_{ik} \tag{39}$$

is an entropy-type inequality

$$\partial_t |Q| + \partial_m v_m |Q|) = \epsilon \frac{|Q| \partial_{kk}}{htr\boldsymbol{P}} \partial_m q_i (E_{q_i q_j}) \partial_m q_j \geq 0, with \{x, y\} \in \{1, 2, 3\}. \tag{40}$$

Proof. Applying Jacobi identity (16) to equation (39), we will get

$$\partial_t |Q| + |Q| Q^{-1}_{ki} v_m \partial_m Q_{ik} + |Q| Q^{-1}_{ki} (\partial_m v_i) Q_{mk} = |Q| Q^{-1}_{ki} T_{ik} \tag{41}$$

$$\Longrightarrow \partial_t |Q| + \partial_m (v_m |Q|) = |Q| Q^{-1}_{ki} T_{ik} \tag{42}$$

$$|Q| Q^{-1}_{ki} T_{ik} = \epsilon \frac{|Q| Q^{-1}_{ki} Q_{ki}}{htr\mathbf{P}} \partial_m q_i \mathcal{E}_{q_i q_j} \partial_m q_j = \epsilon \frac{|Q| \partial_{kk}}{htr\mathbf{P}} \partial_m q_i \mathcal{E}_{q_i q_j} \partial_m q_j \geq 0 \tag{43}$$

Thus, one obtains the following entropy-type inequality associated with the system (32)-(35):

$$\partial_t |Q| + \partial_m v_m |Q|) = \epsilon \frac{|Q| \partial_{kk}}{htr\mathbf{P}} \partial_m q_i (E_{q_i q_j}) \partial_m q_j \geq 0 \tag{44}$$

□

3 Magnetohydrodynamics (MHD)

3.1 Introduction

In 1961, Godunov published his groundbreaking paper "An interesting class of quasilinear systems," in which he discovered the connection between symmetric hyperbolicity in the sense of Friedrichs and thermodynamic compatibility (SHTC), ten years before Friedrichs and Lax, who independently rediscovered the same connection again in 1971[2]. In a subsequent series of papers, Godunov and Romenski carried out further research on this link between symmetric hyperbolicity and thermodynamic compatibility and generalized the seminal idea of Godunov to the more general SHTC framework of symmetric hyperbolic and thermodynamically compatible systems, which includes not only the compressible Euler equations of gas dynamics but also the magnetohydrodynamics (MHD) equations and the equations of nonlinear hyperelasticity[1].

Here, a family of semidiscrete and fully discrete finite volume schemes for overdetermined, hyperbolic, and thermodynamically compatible PDE systems in various dimensions is studied. In particular, we consider the Euler equations of magnetodynamics (MHD), with suitable relaxation of some source terms. SHTC systems can go beyond classical mechanics. Despite the mathematical beauty and rigor of the SHTC framework, up to now it has not been carried much over to the discrete level.

4 Problem Statement

The main aim is to mimic the SHTC (symmetric hyperbolic thermodynamic compatible) framework also on the discrete level by directly discretizing the entropy inequality instead of the total energy conservation law, while the total energy conservation is obtained via an appropriate linear combination as a consequence of the thermodynamically compatible discretization of all equations. Firstly, the system is studied in 1D in a gravity-free space with zero viscosity and zero additional fluxes. And then, it is further taken to multi-dimension with the inclusion of acceleration due to gravity, viscosity terms, and various additional fluxes.

5 Key Terms

5.1 Godunov form of hyperbolic equations

Following the classical Finite-volume method framework, we seek to track a finite set of discrete unknowns, $Q_i^n = \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} q(t^n, x)dx$ where $x_{i-\frac{1}{2}} = x_{low} + (i-\frac{1}{2})\Delta x$ and, $t^n = n\Delta t$ form a discrete set of points for the hyperbolic problem: $q_t + (f(q))_x = 0$, where indices t and x indicate the derivations in time and space, respectively. If we integrate a hyperbolic problem over a control volume, we obtain a method of lines(MOL) formulation for the spatial cell averages. Godunov's method replaces the time integral of each $\int_{t^n}^{t^n+1} f\left(q(t, x_{i-\frac{1}{2}})\right) dt$, using forward Euler method.

5.2 Forward Euler Method

Let's denote the time at the n^{th} time-step by t_n and the computed solution at the nth time-step by y_n, i.e., $y_n \equiv y(t = t_n)$. The step size h (assumed to be constant for the sake of simplicity) is then given by $h = t_n - t_{n-1}$. Given (t_n, y_n), the forward Euler method (FE) computes y_{n+1} as $y_{n+1} = y_n + hf(x_n, y_n)$[6].

5.3 SHTC

Symmetric and Hyperbolic Thermodynamically Compatible systems are a class of systems of quasilinear conservation laws that every closed system owns the additional conservation law (the analog of the first law of thermodynamics) and can be reduced to the symmetric hyperbolic form.

5.4 Numerical Quadrature Rule

Quadrature refers to any method for numerically approximating the value of a definite $\int_b^a f(x)dx$. The goal is to attain a given level of precision with the fewest possible function evaluations. Ex- Trapezoidal rule, Simpson rule, etc. [4]

5.5 Primitive and Conservative Forms

In terms of programming convenience, the non-conservation form is the better of the two. It is easier to program because the equations are solved using the primitive variables (ρ, v, T) and their values can be obtained directly.
However, in the conservation form, the equations are expressed in flux variables that need to be modified in terms of solution vectors. The equations are solved for the solution vectors, and then the primitive variables are determined from them. This adds a fair amount of complexity while solving the governing equations in conservation form. [3]

5.6 Riemann Problems

A Riemann problem in the theory of hyperbolic equations is a problem in which the initial state of the system is defined as:

$$q(x, t = 0) = \begin{cases} q_L & \text{for } x \leq 0 \\ q_R & \text{for } x > 0 \end{cases} \tag{45}$$

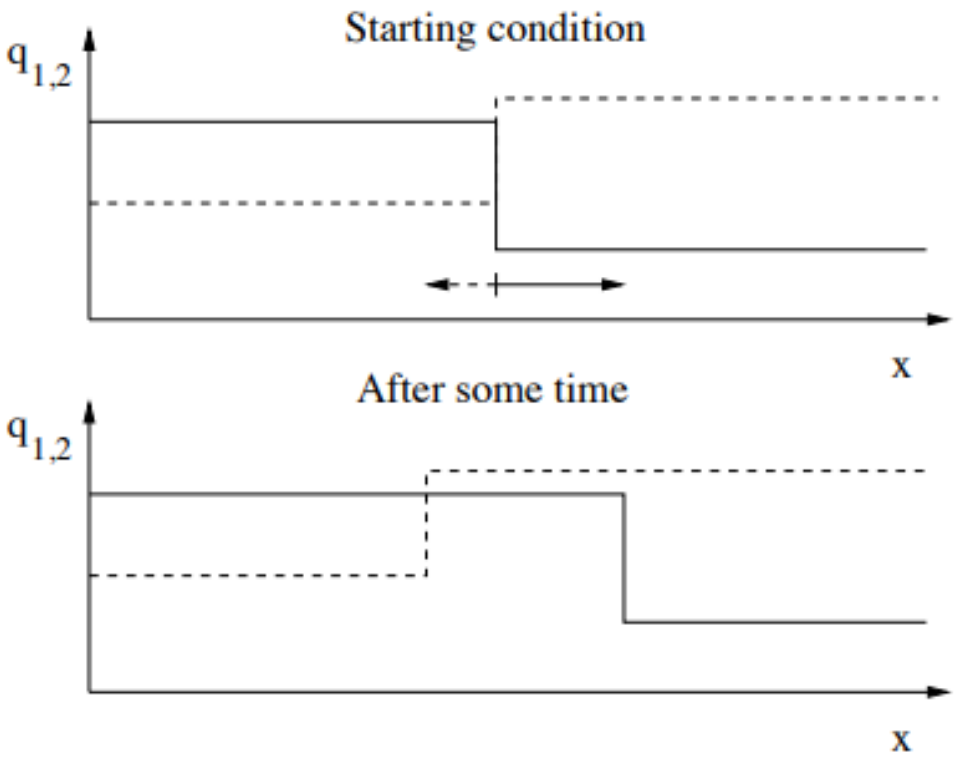

Figure 1: Starting Condition and Condition after sometime

Hydrodynamic problems such as *shock tube tests* are used to test the performance of numerical hydrodynamics algorithms.

5.7 Periodic Boundary Conditions

Periodic boundary conditions (PBCs) are a set of boundary conditions often chosen for approximating an extensive (infinite) system using a small part called a unit cell. PBCs are often used in computer

simulations and mathematical models. An object which has passed through one face of the simulation box should re-enter through the opposite face—or its image should do it.

5.8 Courant Number

The Courant number is a dimensionless value representing the time a particle stays in one cell of the mesh. The derivation of the CFL condition leads to the formula for the Courant number and is given by:

$$C = u\frac{\Delta t}{\Delta x}$$

where C is the Courant number, u is velocity magnitude, Δt is time step size and Δx is the length between mesh elements. It must be below 1 and ideally should be 0.7-0.8.

6 Thermodynamically Compatible Finite Volume Scheme

6.1 Governing Equations

The governing PDE system in one dimension is as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v)}{\partial x} = 0 \tag{46}$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial(\rho v^2 + p)}{\partial x} = 0 \tag{47}$$

$$\frac{\partial \rho S}{\partial t} + \frac{\partial \rho S v}{\partial x} = 0 \tag{48}$$

$$\frac{\partial \mathcal{E}}{\partial t} + \frac{\partial(\mathcal{E} v + p v)}{\partial x} = 0 \tag{49}$$

The system described here represents the Euler subsystem in one dimension in the gravity-free, non-viscous system with no additional fluxes.

6.2 Some terms related to the above PDE

Density is represented by ρ while S is the entropy involved, and E is the specific total energy. Here, $\mathcal{E} = \rho E = \mathcal{E}_1 + \mathcal{E}_2$ is the total energy potential with $\mathcal{E}_i = \rho E_i$.
The two contributors to the total energy density are

$$\mathcal{E}_1 = \frac{\rho^\gamma}{\gamma - 1} e^{S/c_v}, \quad \mathcal{E}_2 = \frac{1}{2}\rho v^2 \tag{50}$$

We will use the notations $\partial_p = \frac{\partial}{\partial p}$ and $\partial^2_{pq} = \frac{\partial^2}{\partial p \partial q}$ for the first and second partial derivatives w.r.t. generic coordinates or quantities p and q, which may also be vectors or components of a vector. we use lower case subscripts, i, j, k, for tensor indices, while lower case superscripts, ℓ, refer to the spatial discretization index. We denote the spatial control volumes in 1D by $\Omega^\ell = [x^{\ell-\frac{1}{2}}, x^{\ell+\frac{1}{2}}]$ and $\Delta x = x^{\ell+\frac{1}{2}} - x^{\ell-\frac{1}{2}}$ is the uniform mesh spacing.

$\mathbf{q} = \{q_i\} = (\rho, \rho v, \rho S)^T$ denotes the state vector. The thermodynamic dual variable $\mathbf{p} = \mathcal{E}_\mathbf{q} = (r, v, T)^T$ along with

$$r = \partial_\rho \mathcal{E}, \quad v = \partial_{\rho v}\mathcal{E}, \quad T = \partial_{\rho S}\mathcal{E} \tag{51}$$

Where T is the temperature.

Gamma(γ) is the ratio of the specific heat at constant pressure(c_p) to the specific heat at constant volume(c_v). The purely hydrodynamic pressure is defined as $p = \rho^2 \frac{\partial E}{\partial \rho}$, where E is the specific total energy. Also,

$$S = \ln\left(\frac{p}{\rho^\gamma}\right), \quad \mathcal{E} = \frac{p}{\gamma - 1} + \frac{1}{2}\rho v^2 \tag{52}$$

6.3 Energy Equation as a Consequence of the above three equations

We will see that equation (4) is a consequence of equation (1)-(3). Firstly, using (2), we get

$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial\left(\rho v^2 + p\right)}{\partial x} = 0$$

$$\implies v\frac{\partial \rho}{\partial t} + v\frac{\partial(\rho v)}{\partial x} + \rho\frac{\partial v}{\partial t} + \rho v\frac{\partial(v)}{\partial x} + \frac{\partial p}{\partial x} = 0$$

$$\implies \rho\frac{\partial v}{\partial t} + \rho v\frac{\partial(v)}{\partial x} + \frac{\partial p}{\partial x} = 0 \quad \text{Using(1)} \tag{53}$$

From (7), we get

$$S = \ln(p) - \gamma\ln(\rho)$$

$$\frac{\partial S}{\partial t} = \frac{\frac{\partial p}{\partial t}}{p} - \frac{\gamma}{\rho}\frac{\partial \rho}{\partial t}, \quad \frac{\partial S}{\partial x} = \frac{\frac{\partial p}{\partial x}}{p} - \frac{\gamma}{\rho}\frac{\partial \rho}{\partial x}$$

Using (3),

$$S\frac{\partial \rho}{\partial t} + S\frac{\partial \rho v}{\partial x} + \rho\frac{\partial S}{\partial t} + \rho v\frac{\partial S}{\partial x} = 0$$

$$\frac{1}{p}\left(\frac{\partial p}{\partial t} + v\frac{\partial \rho}{\partial x}\right) - \frac{\gamma}{\rho}\left(\frac{\partial \rho}{\partial t} + v\frac{\partial \rho}{\partial x}\right) = 0$$

Using (1), we get the following

$$\frac{\partial p}{\partial t} + v\frac{\partial p}{\partial x} + \gamma p\frac{\partial v}{\partial x} = 0 \tag{54}$$

We have,

$$\mathcal{E} + p = \frac{\gamma p}{\gamma - 1} + \frac{1}{2}\rho v^2$$

Then,

$$\frac{\partial \mathcal{E}}{\partial t} + \frac{\partial(\mathcal{E}v + pv)}{\partial x}$$

$$= \frac{\partial\left(\frac{p}{\rho^{\gamma-1}} + \frac{1}{2}\rho v^2\right)}{\partial t} + \frac{\partial\left(\frac{\gamma p v}{\rho^{\gamma-1}} + \frac{1}{2}\rho v^3\right)}{\partial x}$$

$$= \frac{1}{\rho^{\gamma-1}}\frac{\partial p}{\partial t} + \frac{\gamma p}{\gamma-1}\frac{\partial v}{\partial x} + \frac{\gamma v}{\gamma-1}\frac{\partial p}{\partial x} + \rho v\frac{\partial v}{\partial t} + \frac{v^2}{2}\left(\frac{\partial \rho}{\partial t} + v\frac{\partial \rho}{\partial x} + \rho\frac{\partial v}{\partial x}\right) + \rho v^2\frac{\partial v}{\partial x}$$

By using (8) and (1), we have the following

$$= -\frac{v\frac{\partial p}{\partial x}}{\gamma-1} + \frac{v\gamma\frac{\partial p}{\partial x}}{\gamma-1} + \rho v\frac{\partial v}{\partial t} + \rho v^2\frac{\partial v}{\partial x}$$

Now, making use of the (8), we conclude

$$= v\left(\frac{\partial p}{\partial x} + \rho v\frac{\partial v}{\partial x} + \rho\frac{\partial v}{\partial t}\right) = 0$$

6.4 Semi-discrete Godunov formalism for the Euler System

The generating potential, L, is the Legendre transform of the total energy density. It is only related to one of the Euler subsystems, i.e., $\mathcal{E} = \mathcal{E}_1 + \mathcal{E}_2$ and is defined as

$$L = \mathbf{p} \cdot \mathbf{q} - \mathcal{E} \tag{55}$$

$$\implies L = \rho r + \rho v^2 + \rho ST - \frac{p}{\gamma - 1} - \frac{1}{2}\rho v^2 = \rho r + \frac{1}{2}\rho v^2 + \rho ST - \frac{p}{\gamma - 1}$$

We take,

$$\boxed{\mathbf{q} = (\rho, \rho v, \rho S)^T}$$

$$\mathcal{E} = \frac{p}{\gamma - 1} + \frac{1}{2}\rho v^2$$

$$S = ln\left(\frac{p}{\rho^\gamma}\right)$$

Thus,

$$\mathcal{E} = \frac{\rho^\gamma}{\gamma - 1}e^S + \frac{1}{2}\rho v^2$$

6.4.1 Evaluation of p:

$$\mathbf{p} = \left(\frac{\partial \mathcal{E}}{\partial \rho}, \frac{\partial \mathcal{E}}{\partial \rho v}, \frac{\partial \mathcal{E}}{\partial \rho S}\right)^T$$

Now, let us take

$$\rho = m_1, \quad \rho v = m_2, \quad \rho S = m_3$$

Then,

$$\mathcal{E} = \frac{1}{\gamma - 1}m_1^\gamma e^{\frac{m_3}{m_1}} + \frac{1}{2}\frac{m_2^2}{m_1}$$

$$\frac{\partial \mathcal{E}}{\partial m_1} = \frac{\gamma}{\gamma - 1}m_1^{\gamma-1}e^{\frac{m_3}{m_1}} + \frac{1}{\gamma}m_1^\gamma e^{\frac{m_3}{m_1}}\left(\frac{-m_3}{m_1^2}\right) + \frac{1}{2}(-1)\frac{m_2^2}{m_1^2}$$

$$\frac{\partial \mathcal{E}}{\partial m_1} = \frac{\gamma}{\gamma - 1}\rho^{\gamma-1}e^S + \frac{1}{\gamma - 1}\rho^\gamma e^S\left(-\frac{S}{\rho} - \frac{1}{2}\frac{\rho^2 v^2}{\rho^2}\right)$$

$$= \frac{\rho^{\gamma-1}}{\gamma - 1}e^S(\gamma - S) - \frac{1}{2}v^2$$

$$\frac{\partial \mathcal{E}}{\partial m_2} = \frac{1}{2}2\frac{m_2}{m_1} = v$$

$$\frac{\partial \mathcal{E}}{\partial m_3} = \frac{m_1^\gamma}{\gamma - 1}e^{\frac{m_3}{m_1}}\frac{1}{m_3}$$

$$= \frac{\rho^{\gamma-1}}{\gamma - 1}e^S$$

So,

$$\boxed{\mathbf{p} = \left(\frac{\rho^{\gamma-1}}{\gamma - 1}e^S(\gamma - S) - \frac{1}{2}v^2, v, \frac{\rho^{\gamma-1}}{\gamma - 1}e^S\right)^T}$$

6.4.2 Evaluation of L:

We know that,

$$L = \mathbf{p}\cdot\mathbf{q} - \mathcal{E}$$

$$= \frac{\rho^\gamma}{\gamma-1}e^S(\gamma - S) - \frac{1}{2}\rho v^2 + \rho v^2 + \frac{\rho^\gamma}{\gamma-1}Se^S - \frac{\rho^\gamma e^S}{\gamma-1}\gamma - \frac{\rho^\gamma}{\gamma-1}e^S$$

$$\implies \boxed{L = \rho^\gamma e^S}$$

Thus, we have

$$\boxed{vL = v\rho^\gamma e^S}$$

6.4.3 Evaluation of f:

$$\mathbf{f} = \partial_{\mathbf{p}}(v\rho^\gamma e^S)$$

Let us consider

$$m_1 = \frac{\rho^{\gamma-1}}{\gamma-1}e^S(\gamma - S) - \frac{1}{2}v^2, \quad m_2 = v, \quad m_3 = \frac{\rho^{\gamma-1}}{\gamma-1}e^S$$

Clearly,

$$m_1 = \frac{\rho^{\gamma-1}}{\gamma-1}e^S(\gamma - S) - \frac{1}{2}m_2^2$$

$$\implies m_1 + \frac{1}{2}m_2^2 = m_3(\gamma - S)$$

$$\gamma - S = \frac{m_1}{m_3} + \frac{1}{2}\frac{m_2^2}{m_3}$$

$$S = \gamma - \frac{m_1}{m_3} - \frac{1}{2}\frac{m_2^2}{m_3}$$

$$m_3 = \frac{\rho^{\gamma-1}}{\gamma-1}e^{\gamma - \frac{m_1}{m_3} - \frac{1}{2}\frac{m_2^2}{m_3}}$$

$$\implies \rho^{\gamma-1} = (\gamma-1)m_3 e^{\frac{m_1}{m_3} + \frac{1}{2}\frac{m_2^2}{m_3} - \gamma}$$

$$\implies \rho = ((\gamma-1)m_3)^{\frac{1}{\gamma-1}} e^{\frac{m_1}{(\gamma-1)m_3} + \frac{m_2^2}{2m_3(\gamma-1)} - \frac{\gamma}{\gamma-1}}$$

Now, we have the following term

$$v\rho^\gamma S = m_2((\gamma-1)m_3)^{\frac{\gamma}{\gamma-1}} e^{\frac{\gamma m_1}{(\gamma-1)m_3} + \frac{\gamma m_2^2}{2m_3(\gamma-1)} - \frac{\gamma^2}{\gamma-1}} e^{\gamma - \frac{m_1}{m_3} - \frac{1}{2}\frac{m_2^2}{m_3}}$$

$$= m_2((\gamma-1)m_3)^{\frac{\gamma}{\gamma-1}} e^{\frac{m_1}{(\gamma-1)m_3} + \frac{m_2^2}{2m_3(\gamma-1)} - \frac{\gamma}{\gamma-1}}$$

Differentiating it with respect to the first term, i.e., m_1, we get

$$\frac{\partial(v\rho^\gamma e^S)}{\partial m_1} = \frac{1}{(\gamma-1)m_3} m_2((\gamma-1)m_3)^{\frac{\gamma}{\gamma-1}} e^{\frac{m_1}{(\gamma-1)m_3} + \frac{m_2^2}{2m_3(\gamma-1)} - \frac{\gamma}{\gamma-1}}$$

$$= v(\rho^{\gamma-1}e^S)^{\frac{\gamma}{\gamma-1}} e^{\frac{-S}{\gamma-1}} \frac{1}{\rho^{\gamma-1}e^S}$$

$$= v\frac{\rho^\gamma}{\rho\gamma - 1} = \rho v$$

Differentiating it with respect to the second term, i.e., m_2, we get

$$\frac{\partial(v\rho^\gamma e^S)}{\partial m_2}$$

$$= ((\gamma-1)m_3)^{\frac{\gamma}{\gamma-1}} e^{\frac{m_1}{(\gamma-1)m_3}+\frac{m_2^2}{2m_3(\gamma-1)}-\frac{\gamma}{\gamma-1}} + m_2((\gamma-1)m_3)^{\frac{\gamma}{\gamma-1}} e^{\frac{m_1}{(\gamma-1)m_3}+\frac{m_2^2}{2m_3(\gamma-1)}-\frac{\gamma}{\gamma-1}} \frac{m_2}{(\gamma-1)m_3}$$

$$(\rho^{\gamma-1}e^S)^{\frac{\gamma}{\gamma-1}} e^{\frac{-S}{\gamma-1}} + v((\gamma-1)m_3)^{\frac{\gamma}{\gamma-1}} e^{\frac{m_1}{(\gamma-1)m_3}+\frac{m_2^2}{2m_3(\gamma-1)}-\frac{\gamma}{\gamma-1}} \frac{v}{\rho^{\gamma-1}e^S}$$

$$= \rho^\gamma e^S + v\frac{\rho^\gamma}{\rho^{\gamma-1}}v$$

$$= \rho^\gamma e^S + \rho v^2$$

$$= p + \rho v^2$$

Differentiating with respect to the third variable, i.e., m_3, we get

$$\frac{\partial(v\rho^\gamma e^S)}{\partial m_3}$$

$$= \gamma m_2 \left((\gamma-1)m_3\right)^{\frac{\gamma}{\gamma-1}} e^{\frac{m_1}{(\gamma-1)m_3}+\frac{m_2^2}{2m_3(\gamma-1)}-\frac{\gamma}{\gamma-1}} + \frac{1}{\gamma-1}\left(\frac{-m_1}{m_3^2} - \frac{1}{2}\frac{m_2^2}{m_3^2}\right) m_2 \left((\gamma-1)m_3\right)^{\frac{\gamma}{\gamma-1}} e^{\frac{m_1}{(\gamma-1)m_3}+\frac{m_2^2}{2m_3(\gamma-1)}-\frac{\gamma}{\gamma-1}}$$

$$= \gamma v(\rho^{\gamma-1}e^S)^{\frac{1}{\gamma-1}} e^{\frac{-S}{\gamma-1}} + \frac{1}{\gamma-1}\frac{-m_1-m_2^2}{2m_3^2} v(\rho^{\gamma-1}e^S)^{\frac{\gamma}{\gamma-1}} e^{\frac{-S}{\gamma-1}}$$

$$= \gamma v\rho e^{S(\frac{1}{2}-\frac{1}{2})} + \frac{1}{\gamma-1} v\rho^\gamma e^S \left(\frac{-\rho^{\gamma-1}e^S(\gamma-S)(\gamma-1)^2}{(\gamma-1)\rho^{2(\gamma-1)}e^{2S}}\right)$$

$$= \gamma v\rho + \rho v\left(-\gamma + S\right)$$

$$= \rho v S$$

Therefore, we have the following exact form of $\mathbf{f}$:

$$\boxed{\mathbf{f} = \left(\rho v, p + \rho v^2, \rho v S\right)}$$

Clearly, now the equation

$$\boxed{\mathbf{q}_t + \mathbf{f}_x = 0}$$

gives the equations for the Euler subsystem.

6.4.4 Evaluation of $F_{\mathbf{G}}$:

Now, we have,

$$F_G = \mathbf{p}\cdot\mathbf{f} - vL$$

$$\implies F_G = \frac{\rho^\gamma}{\gamma-1} v e^S(\gamma - S) - \frac{1}{2}\rho v^3 + \rho^\gamma v e^S + \rho v^3 + \frac{\rho^\gamma}{\gamma-1} v S e^S$$

$$\implies F_G = \frac{\rho^\gamma}{\gamma-1} v e^S \gamma + \frac{1}{2}\rho v^3 + \rho^\gamma v e^S$$

Thus, we have the following value of F_G:

$$\boxed{F_G = \rho^\gamma v e^S \left(\frac{2\gamma-1}{\gamma-1}\right) + \frac{1}{2}\rho v^3}$$

The Godunov form of the inviscid Euler subsystems is as follows:

$$\mathbf{q} = \partial_{\mathbf{p}} L, \quad \mathbf{p} = \partial_{\mathbf{q}} \mathcal{E}, \quad \mathbf{f} = \partial_{\mathbf{p}}(vL), \quad F_G = \mathbf{p}\cdot\mathbf{f} - vL \tag{56}$$

$$(\partial_{\mathbf{p}} L)_t + \partial_x(\partial_{\mathbf{p}}(vL)) = 0 \tag{57}$$

A semi-discrete finite volume scheme for (12) is as follows:

$$\frac{d}{dt}\mathbf{q}^{\ell} = -\frac{\mathbf{f}^{\ell+\frac{1}{2}} - \mathbf{f}^{\ell-\frac{1}{2}}}{\Delta x} = -\frac{(\mathbf{f}^{\ell+\frac{1}{2}} - \mathbf{f}^{\ell}) - (\mathbf{f}^{\ell-\frac{1}{2}} - \mathbf{f}^{\ell})}{\Delta x} \tag{58}$$

with $\mathbf{f}^{\ell} = \mathbf{f}(\mathbf{q}^{\ell})$ and $\mathbf{f}(\mathbf{q}) = (\rho v, \rho v^2 + p, \rho S v)^T$, the fluxes of the Euler subsystem and $F_G = v(\mathcal{E}_1 + \mathcal{E}_2 + p)$ the total associated energy flux.

In order to obtain a discrete total energy conservation law as a consequence of the discretization of (1)-(3), we firstly compute the dot product of the discrete dual variables, $\mathbf{p}^{\ell} = \partial_{\mathbf{q}}\mathcal{E}(\mathbf{q}^{\ell})$, with the semi-discrete scheme:

$$\mathbf{p}^{\ell} \cdot \frac{d}{dt}\mathbf{q}^{\ell} = \frac{d}{dt}\mathcal{E}^{\ell} = -\mathbf{p}^{\ell} \cdot \frac{(\mathbf{f}^{\ell+\frac{1}{2}} - \mathbf{f}^{\ell}) - (\mathbf{f}^{\ell} - \mathbf{f}^{\ell-\frac{1}{2}})}{\Delta x} = -\frac{D_{\mathcal{E}}^{\ell-\frac{1}{2},-} + D_{\mathcal{E}}^{\ell-\frac{1}{2},+}}{\Delta x} \tag{59}$$

The energy fluctuation is defined as $D_{\mathcal{E}}^{\ell-\frac{1}{2},-} = \mathbf{p}^{\ell} \cdot (\mathbf{f}^{\ell+\frac{1}{2}} - \mathbf{f}^{\ell}), D_{\mathcal{E}}^{\ell-\frac{1}{2},+} = \mathbf{p}^{\ell} \cdot (\mathbf{f}^{\ell} - \mathbf{f}^{\ell-\frac{1}{2}})$, which must satisfy the consistency property (i.e., the change in flux is equal to the total change in energy density)

$$D_{\mathcal{E}}^{\ell+\frac{1}{2},-} + D_{\mathcal{E}}^{\ell+\frac{1}{2},+} = \mathbf{p}^{\ell} \cdot (\mathbf{f}^{\ell+\frac{1}{2}} - \mathbf{f}^{\ell}) + \mathbf{p}^{\ell+1} \cdot (\mathbf{f}^{\ell+1} - \mathbf{f}^{\ell-\frac{1}{2}}) = F_G^{\ell+1} - F_G^{\ell} \tag{60}$$

in order to obtain a conservative discretization of (4). F_G^{ℓ} is the discrete total energy flux F_G in cell Ω^{ℓ} in the above equation.
Using (55), i.e $f^{l+\frac{1}{2}} = \partial_{\mathbf{p}}(v_1 L)(l + \frac{1}{2})$, we get the following:

$$-\partial_{\mathbf{p}}(vL)^{l+\frac{1}{2}} \cdot (\mathbf{p}^{l+1} - \mathbf{p}^{l}) + \mathbf{p}^{l+1} \cdot f^{l+1} - \mathbf{p}^{l} \cdot f^{l} = \mathbf{p}^{l+1} \cdot f^{l+1} - (vL)^{l+1} - \mathbf{p}^{l} \cdot f^{l} + (vL)^{l}. \tag{61}$$

Also, the numerical flux $f^{l+\frac{1}{2}}$ must verify the Roe-type property,

$$\mathbf{f}^{l+\frac{1}{2}} \cdot (\mathbf{p}^{l+1} - \mathbf{p}^{l}) = \partial_{\mathbf{p}}(vL) \cdot (\mathbf{p}^{l+1} - \mathbf{p}^{l}) = (vL)^{l+1} - (vL)^{l}. \tag{62}$$

Now, we will take into consideration the basic ideas of path conservative schemes, the path integral of the flux $\mathbf{f} = \partial_{\mathbf{p}}(vL)$ satisfy the identity

$$(vL)^{l+1} - (vL)^{l} = \int_{\mathbf{p}^{l}}^{\mathbf{p}^{l+1}} \partial_{\mathbf{p}}(vL) \cdot d\mathbf{p} = \int_0^1 \partial_{\mathbf{p}}(vL) \cdot \frac{\partial \boldsymbol{\psi}}{\partial s} ds, \tag{63}$$

for any path $\boldsymbol{\psi}, s \in [0, 1]$ in phase space. We chose the simple straight line segment path in $\mathbf{p}$ variables, i.e.

$$\boldsymbol{\psi}(s) = \mathbf{p}^{l} + s(\mathbf{p}^{l+1} - \mathbf{p}^{l}), \quad \frac{\partial \boldsymbol{\psi}}{\partial s} = \mathbf{p}^{l+1} - \mathbf{p}^{l}, \quad 0 \le s \le 1. \tag{64}$$

Inserting the segment path (63) in (62) gives us the following:

$$(vL)^{l+1} - (vL)^{l} = \left(\int_0^1 \mathbf{f}(\boldsymbol{\psi}(s)) ds \right) \cdot (\mathbf{p}^{l+1} - \mathbf{p}^{l}). \tag{65}$$

As a result, the thermodynamically compatible numerical flux for the inviscid Euler subsystem

$$\mathbf{f}_{\mathbf{p}}^{l+\frac{1}{2}} = \int_0^1 \mathbf{f}(\boldsymbol{\psi}(s)) ds = \left(f_{\rho}^{l+\frac{1}{2}}, \mathbf{f}_{\rho\mathbf{v}}^{l+\frac{1}{2}}, f_{\rho S}^{l+\frac{1}{2}} \right)^T \tag{66}$$

As we have the exact form of the equations, we can employ them and do the quantitative study on the total energy conservation for the Euler subsystem.

6.5 Numerical Flux

We try to find a numerical flux $\mathbf{f}$ that satisfies

$$\mathbf{f} \cdot [[\mathbf{p}]] = [[pv]] \tag{67}$$

where $[[.]]$ denotes the jump between the two states. We will denote the arithmetic average by an overbar

$$\overline{(.)} = \frac{1}{2}[(.)_l + (.)_r] \tag{68}$$

6.6 Approach

Write all jump terms in terms of jumps in ρ, T, v where $T = \frac{p}{\rho}$. Now, we know that

$$S = ln(p) - \gamma ln(\rho) = ln(\rho) + ln(T) - \gamma ln(\rho) = -(\gamma - 1)ln(\rho) + ln(T) \tag{69}$$

From this, we get

$$[[S]] = -(\gamma - 1)\frac{[[\rho]]}{\hat{\rho}} + \frac{[[T]]}{\hat{T}} \tag{70}$$

Where we define the logarithmic average

$$\hat{\phi} = \frac{[[\phi]]}{[[ln(\phi)]]} \tag{71}$$

Then, we have

$$\begin{aligned}
[[p_1]] &= \frac{\gamma}{\gamma - 1}[[T]] - \frac{1}{\gamma - 1}[[TS]] - \overline{v}[[v]] \\
&= \frac{\gamma - \overline{S}}{\gamma - 1}[[T]] - \frac{\overline{T}}{\gamma - 1}[[S]] - \overline{v}[[v]] \\
&= \left(\frac{\gamma - \overline{S} - \frac{\overline{T}}{\hat{T}}}{\gamma - 1} \right)[[T]] - \overline{v}[[v]] + \frac{\overline{T}}{\hat{\rho}}[[\rho]]
\end{aligned}$$

$$[[p_2]] = [[v]]$$

$$[[p_3]] = \frac{1}{\gamma - 1}[[T]]$$

$$[[pv]] = [[\rho v T]]$$

$$= \overline{\rho v}[[T]] + \overline{T}[[pv]]$$

$$= \overline{\rho v}[[T]] + \overline{T}\overline{\rho}[[v]] + \overline{T}\overline{v}[[\rho]]$$

Thus, finally, we get,

$$f_1 = \hat{\rho}\overline{v}, \quad f_2 = \overline{\rho}\overline{T} + \overline{v}f_1, \quad f_3 = (\gamma - 1)\overline{\rho v} - \left(\gamma - \overline{S} - \frac{\overline{T}}{\hat{T}}\right) f_1 \tag{72}$$

7 Algorithm And Code-Link

7.1 Algorithm

The code has the following structure:

- Discretize the space by creating the numerical grid
- Set the initial conditions
- Main timestep evolution loop
  - Compute the timestep
  - Loop to advance one step (count depends on the number of stages in the integrator)
    - Reconstruct the state to interfaces
    - Find the fluxes through the interface
    - Do a conservative update of the state to the stage
- Output

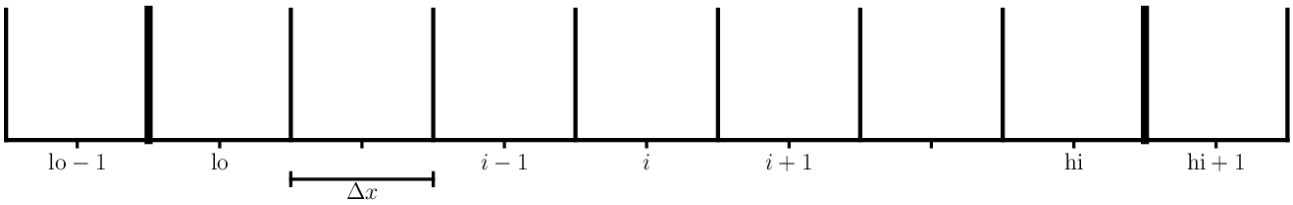

Figure 2: Visual Image of the Grid

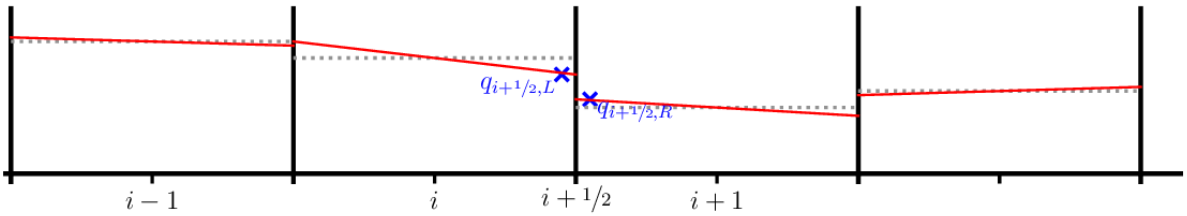

Figure 3: Visual Image of the states at the interfaces

7.2 Implementation Details

We manage our 1-d grid via a class FVGrid. We divide the domain into several zones (or volumes) that will store the state. We traditionally use ghost cells to implement boundary conditions–extra cells added to each end of the domain. We use *lo* and *hi* to refer to our domain's first and last zone. We need to use the cell averages to determine the fluid state on the interfaces. We'll reconstruct the cell averages as piecewise lines that give us the same average in the zone. We then follow these lines to the interfaces to define each interface's left and right states. Usually, we work in terms of the primitive variables, $q = (\rho, u, p)$ So, we first write a routine to do the algebraic transformation from conservative to primitive variables:

$$\rho = \rho$$
$$u = \frac{\rho u}{\rho}$$

$$p = \left((\rho E) - \frac{1}{2} \frac{(\rho u)^2}{\rho} \right) (\gamma - 1)$$

Next, we need a routine to create the interface states. Here we'll construct a slope for each zone, δq, based on the average state in the neighboring zones. This gives us a line representing the value of the fluid state as a function of position in each zone:

$$q_i(x) = \langle q \rangle_i + \frac{\Delta q_i}{\Delta x}(x - x_i)$$

Note that there is a unique $q_i(x)$ for each zone—this is usually called piecewise linear reconstruction. By design, the average of $q_i(x)$ over the zone is the cell average, so it is conservative.

We use this equation for a line to find the fluid state right at the interface. For zone i, the line $q_i(x)$ gives us the right state on the left interface, $q_{i+\frac{1}{2},R}$, and the left state on the right interface, $q_{i+\frac{1}{2},L}$.

There's one additional wrinkle—2^{nd} order codes tend to produce oscillations near discontinuities, so we usually need to limit the slopes, Δq_i , so we don't introduce new minima or maxima in the evolution. We'll use the minmod limiter:

$$\frac{\delta a}{\delta x} = minmod_i \left(\frac{a_i - a_{i-1}}{\Delta x}, \frac{a_{i+1} - a_i}{\Delta x} \right)$$

with

$$minmod(a, b) = \begin{cases} a \text{ if } |a| < |b| \text{ and } a.b > 0 \\ b \text{ if } |a| > |b| \text{ and } a.b > 0 \\ 0 \text{ otherwise} \end{cases}$$

After doing our reconstruction, we are left with a left and right state on an interface. To find the unique fluid state on the interface, we solve a Riemann problem,

$$q_{i+\frac{1}{2}} = \mathcal{R} \left(q_{i+\frac{1}{2},L}, q_{i+\frac{1}{2},R} \right)$$

Once we have the interface state, we can compute the fluxes using this state. Also, the time stamp is calculated as we cannot allow information to move more than one zone per step. The update in the driver code looks like this:

$$U^* = U^n + \frac{\Delta t}{2} A(U^n)$$

$$U^{n+1} = U^n + \Delta t A(U^*)$$

7.3 Code Link

The code is implemented in Python and is available at Code Link

8 Results

The ratio of specific heats of the fluid is chosen to be $\gamma = 1.4$. For all problems, the spatial domain is the interval [0,1] which is discretized with $M = 100$ computing cells. The codes were run on various problems like Sod Problem, Lax Problem [5], etc., with different initial conditions, parameters, and grids.

The initial conditions of the test problems are given in the table below:

Initial Conditions for Various Problems						
Test Name	ρ_L	u_L	p_L	ρ_R	u_R	p_R
Sod Problem	1.0	0.0	1.0	0.125	0.0	0.1
Lax Problem	0.445	0.698	3.528	0.5	0.0	0.571
Strong Shock Problem	1.0	0.0	1000.0	1.0	0.0	0.01
Woodward and Colella Problem	1.0	0.0	0.01	1.0	0.0	100.0

8.1 No Shock Example Problem

We took one example problem with the initial conditions as follows:

$$p = 1$$

$$v = 1$$

$$\rho = 2 + Sin(2\pi x)$$

The exact solution for this problem is

$$\rho = 2 + Sin(2\pi(x - t))$$

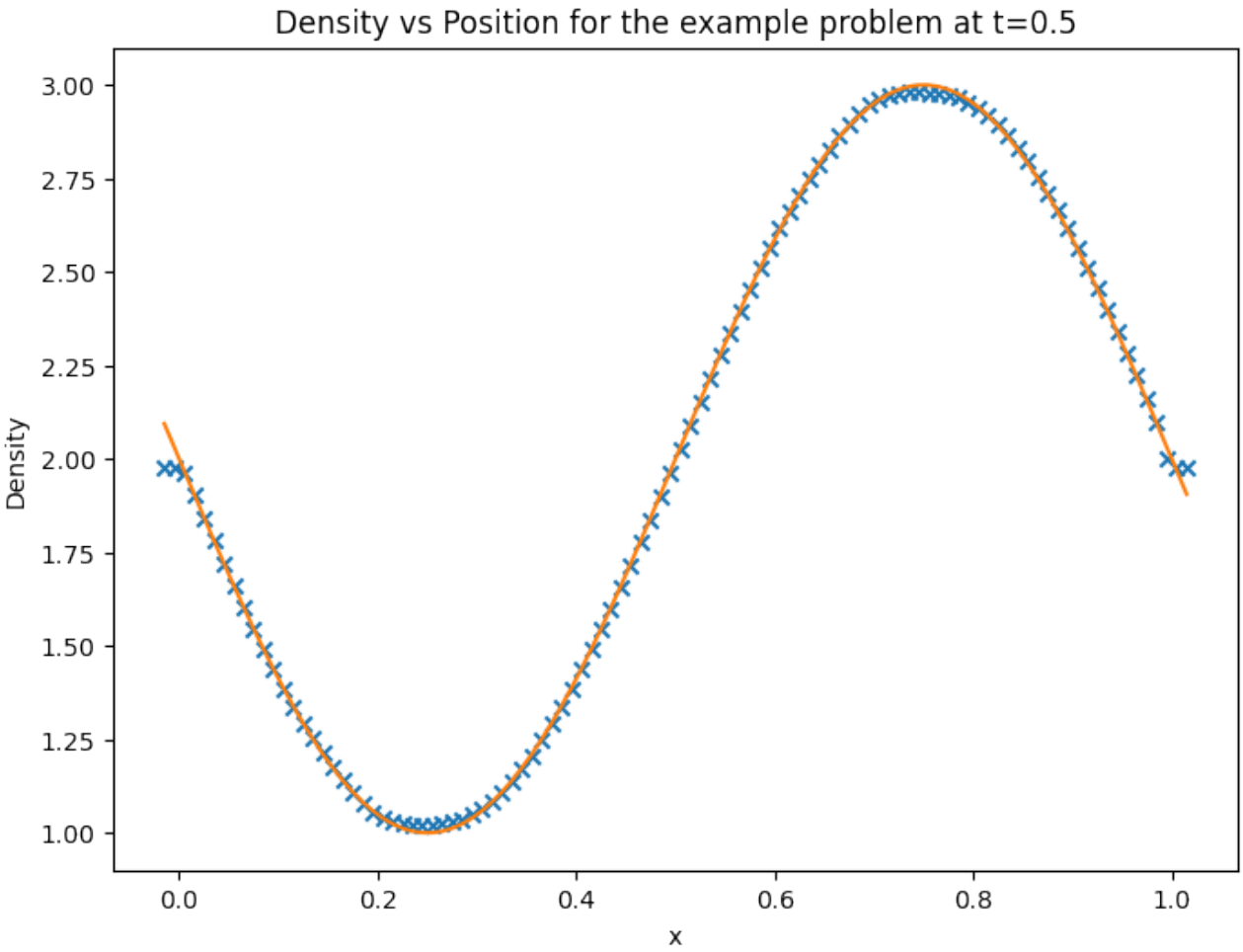

Figure 4: Density vs. Position for the example problem

The solid line represents the exact solution, while the cross-mark represents the solution through our scheme. We can see that our solution matches the exact solution.

8.2 Sod Problem

The Sod problem is a standard test problem consisting of a left and right state separated by an initial discontinuity. As time evolves, a rightward moving shock, contact, and leftward moving rarefaction form. The curve obtained with our scheme matches the exact solution. The plot shown below is drawn for the point of discontinuity $x = 0.5$ at output time 0.15 units:

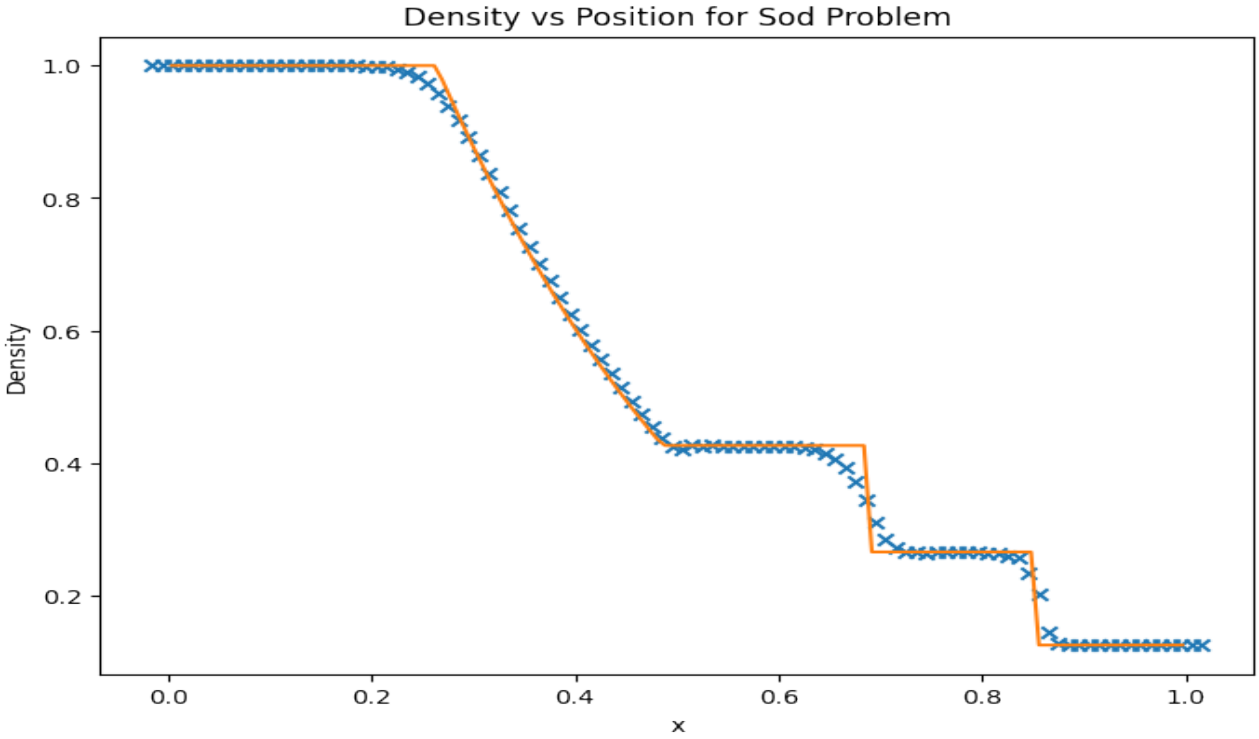

Figure 5: Density vs. Position for the Sod problem

The solid line gives the exact solution, while the solution is obtained through our schemes. We can see that it matches the exact solution.

8.3 Lax Problem

The initial conditions are given in the table above. The plots obtained through our scheme and the exact solution are given below. The plots are drawn for the point of discontinuity $x = 0.5$ at the output time 0.13 units.

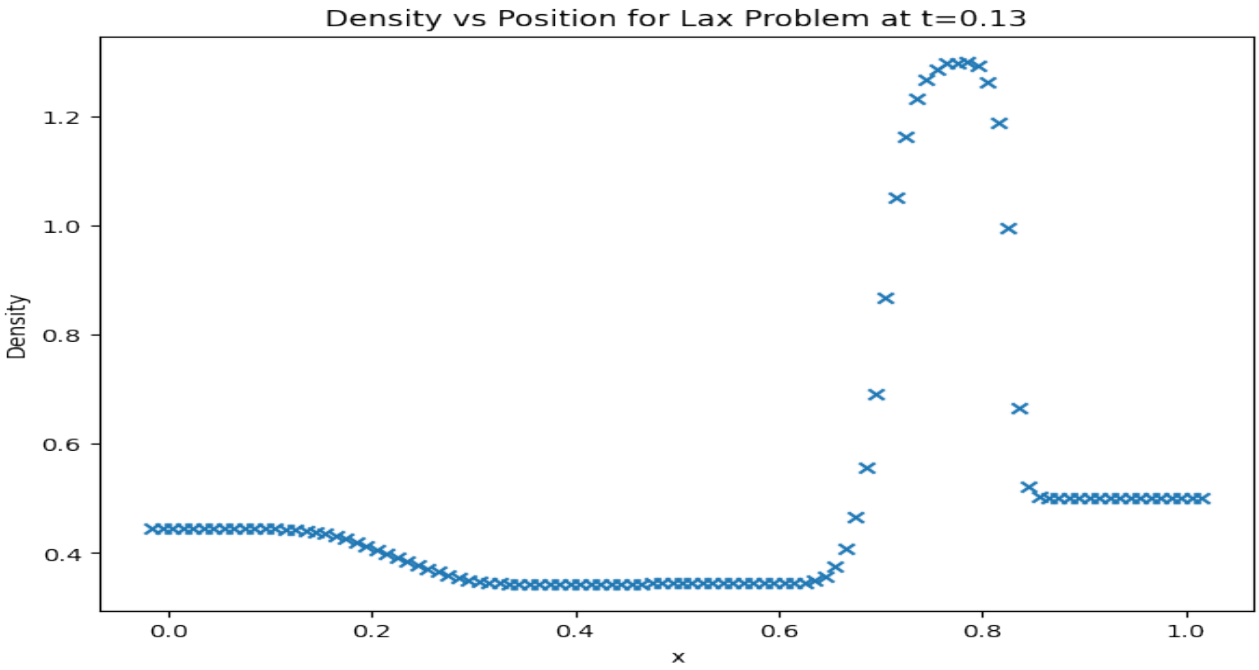

Figure 6: Density vs. Position for the Lax problem

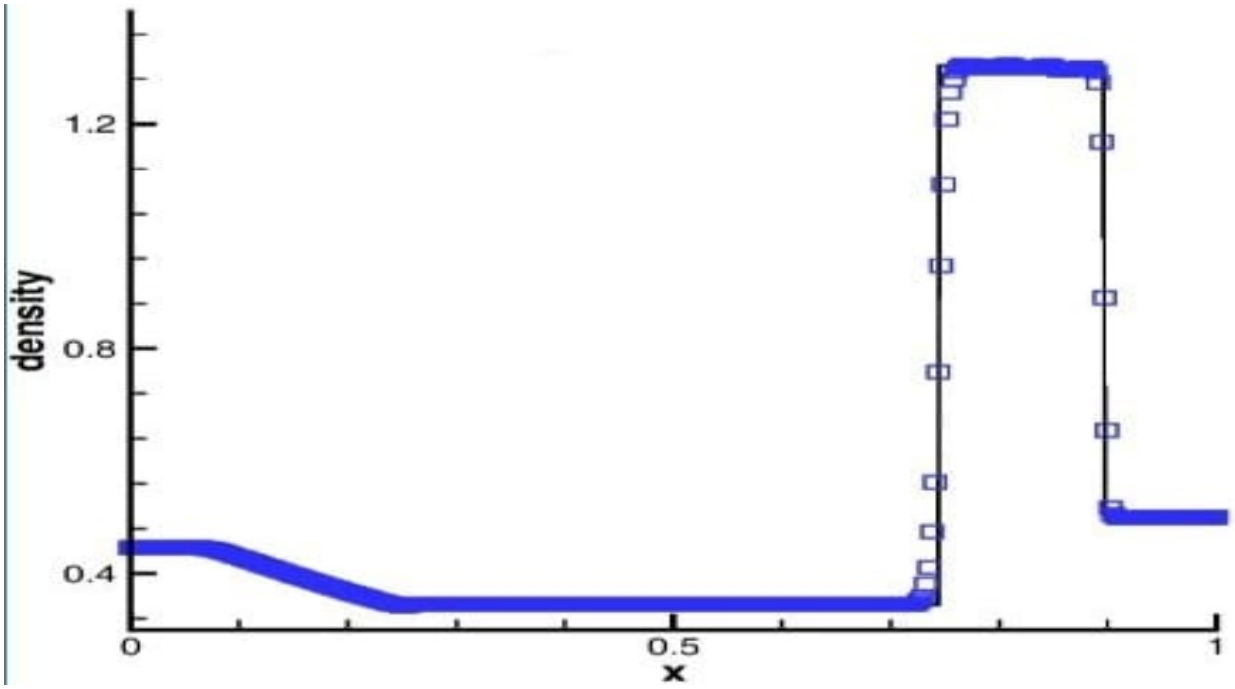

Figure 7: Exact plot of Density vs. Position for the Lax problem

In this case, as well, our scheme matches the exact solution.

8.4 Strong Shock Problem

The above table contains the initial conditions. The plots obtained by our approach, as well as the exact solution, are shown below. The plots are drawn for the point of discontinuity $x = 0.5$ at the output time 0.012 units.

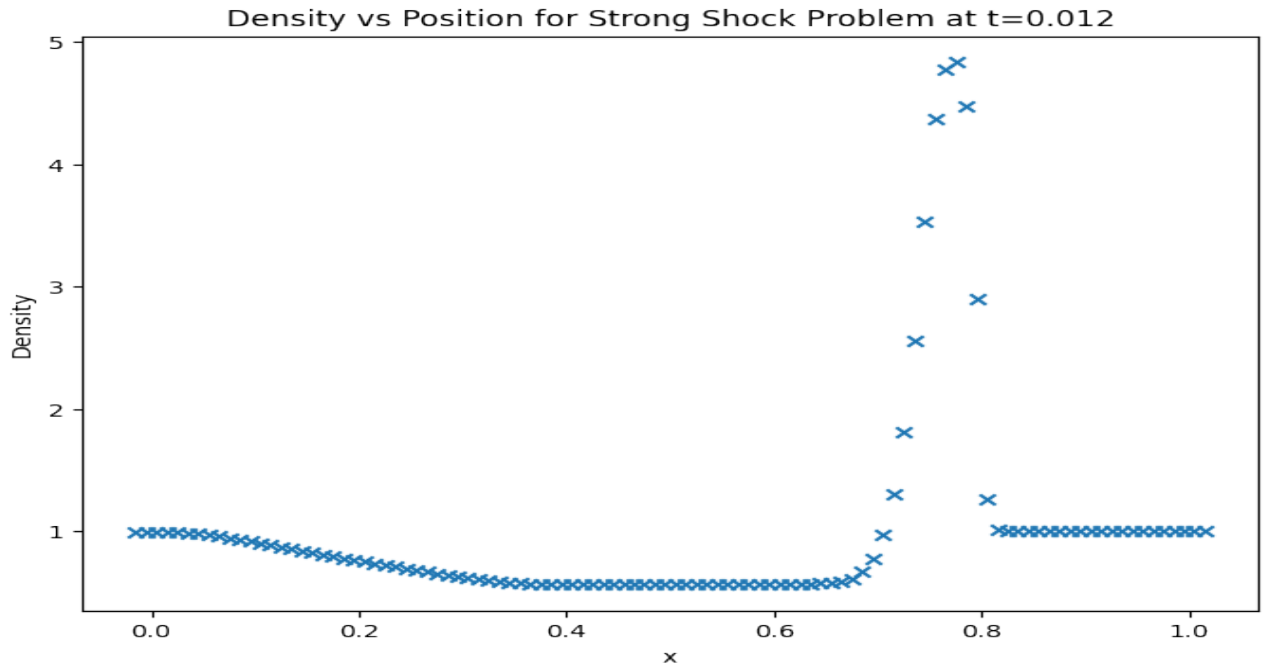

Figure 8: Density vs. Position for the Strong Shock problem

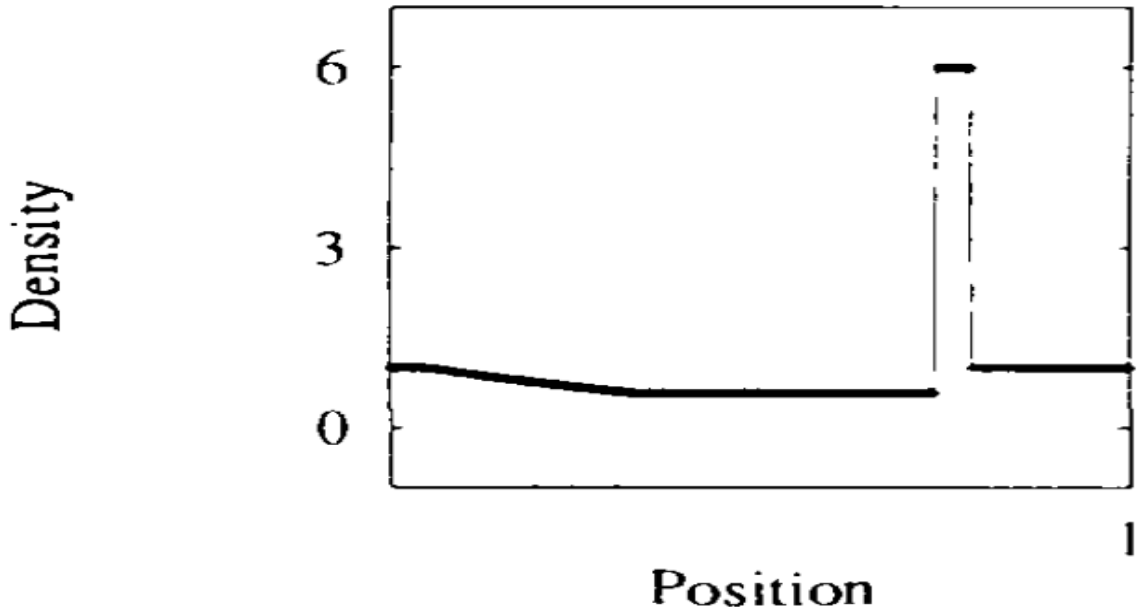

Figure 9: Exact plot of Density vs. Position for the Strong Shock problem

We see that the plot acquired by our approach is identical to the exact solution.

8.5 Woodward and Colella Problem

The starting circumstances are outlined in the table that can be found above. The plots that were generated by our approach, as well as the precise solution, can be found below. The plots are drawn for the point of discontinuity $x = 0.5$ at the output time 0.035 units.

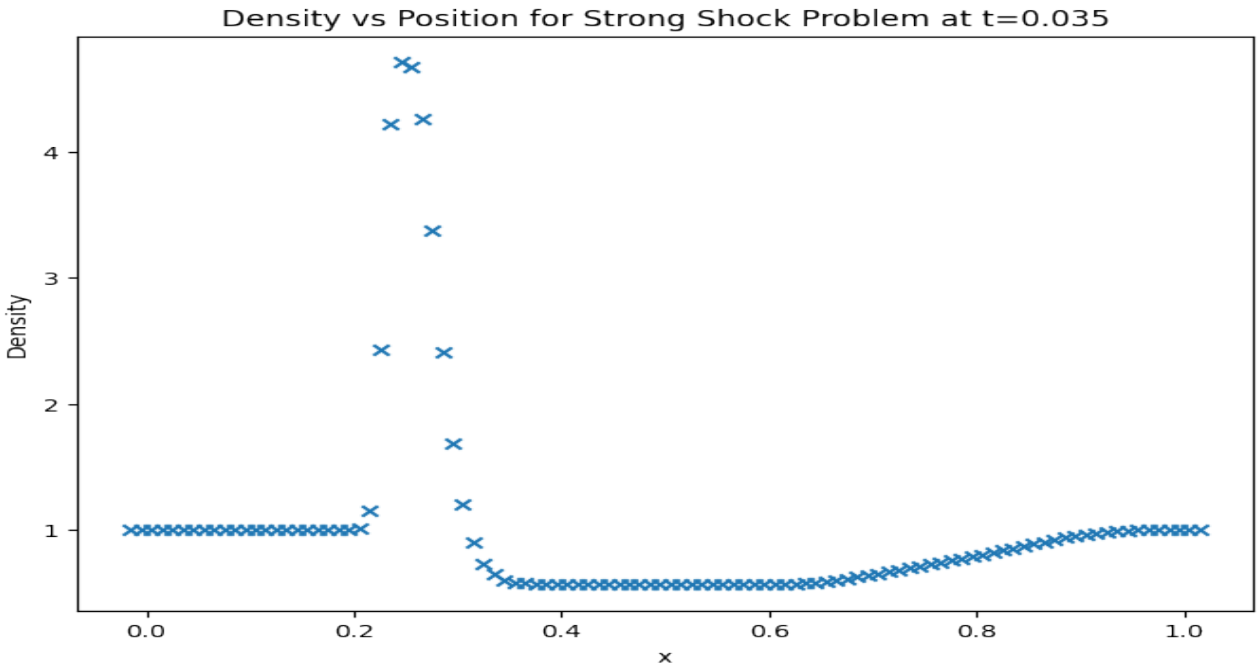

Figure 10: Density vs. Position for the Lax problem

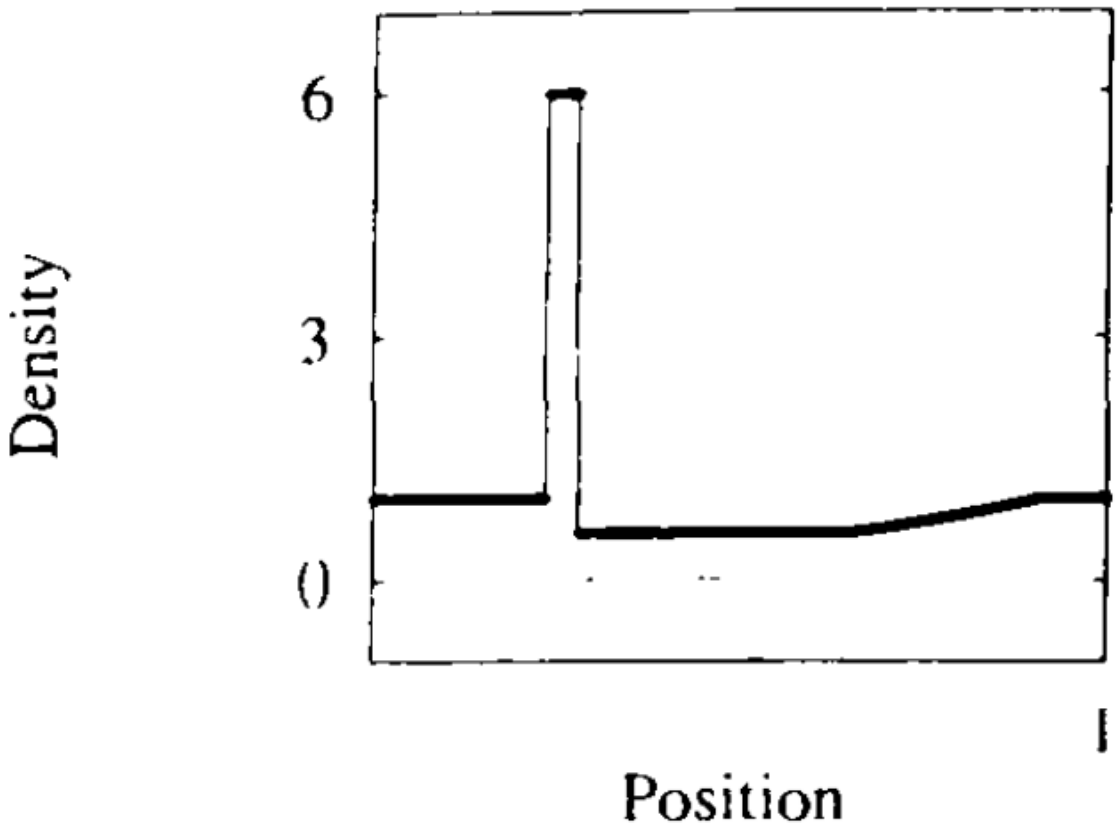

Figure 11: Exact plot of Density vs. Position for the Woodward and Colella problem

Also in this instance, our plan corresponds precisely with the exact solution.
We observe that the numerical solution obtained through our scheme is convergent and consistent with the exact solutions of various test problems.

9 Dissipation Terms

In order to obtain a dissipative thermodynamically compatible scheme, we need to add a compatible numerical dissipation to the inviscid flux derived in the previous section.
We will add an additional dissipative flux and a corresponding entropy production term as follows:

$$\frac{d}{dt}\mathbf{q}^l + \frac{\mathbf{f}^{l+\frac{1}{2}} - \mathbf{f}^{l-\frac{1}{2}}}{\Delta x} = \frac{\mathbf{g}^{l+\frac{1}{2}} - \mathbf{g}^{l-\frac{1}{2}}}{\Delta x} + \mathbf{P}^l \tag{73}$$

The dissipative part of the numerical flux is taken of the form

$$\mathbf{g}^{l+\frac{1}{2}} = \epsilon^{l+\frac{1}{2}} \frac{\Delta \mathbf{q}^{l+\frac{1}{2}}}{\Delta x}, \quad \Delta \mathbf{q}^{l+\frac{1}{2}} = \mathbf{q}^{l+1} - \mathbf{q}^l \tag{74}$$

where the scalar numerical dissipation coefficient can be either taken as a constant, $\epsilon^{l+\frac{1}{2}} = \epsilon$ or of the form

$$\epsilon^{l+\frac{1}{2}} = \frac{1}{2}\left(1 - \phi^{l+\frac{1}{2}}\right) \Delta x s_{max}^{l+\frac{1}{2}} \geq 0 \tag{75}$$

where $s_{max}^{l+\frac{1}{2}}$ is the maximum signal speed at the cell interface (Rusanov flux) and $\phi^{l+\frac{1}{2}}$ is a flux limiter that permits the numerical dissipation to be reduced in smooth regions. We employ the minbee flux limiter in this work, which reads

$$\phi^{l+\frac{1}{2}} = min\left(\phi_-^{l+\frac{1}{2}}, \phi_+^{l+\frac{1}{2}}\right), with \quad \phi_\pm = max\left(0, min\left(1, h_\pm^{l+\frac{1}{2}}\right)\right) \tag{76}$$

where the ratio of density slopes are

$$h_{-}^{l+\frac{1}{2}} = \frac{\rho^{l} - \rho^{l-1}}{\rho^{l+1} - \rho^{l}}, \quad h_{+}^{l+\frac{1}{2}} = \frac{\rho^{l+2} - \rho^{l+1}}{\rho^{l+1} - \rho^{l}} \tag{77}$$

We will now do the dot product of $\mathbf{p}^l$ with the updated equation (including the dissipative flux and entropy production terms), which leads to the following equation:

$$\frac{d\mathcal{E}^l}{dt} + \frac{1}{\Delta x}\left(F_G^{l+\frac{1}{2}} - F_G^{l-\frac{1}{2}}\right) = \frac{1}{\Delta x}\mathbf{p}^l \cdot \left(\mathbf{g}^{l+\frac{1}{2}} - \mathbf{g}^{l-\frac{1}{2}}\right) + \mathbf{p}^l \cdot \mathbf{P}^l \tag{78}$$

using the numerical energy flux derived from the total energy fluctuation at the interface as $F_G^{l+\frac{1}{2}} = D_\epsilon^{l+\frac{1}{2},-} + F_G^l$. Because the thermodynamic compatibility of the left-hand side has already been explored in the previous section, we can now concentrate on the right-hand side of the equation.

$$\mathbf{p}^l \cdot \mathbf{P}^l + \frac{1}{\Delta x}\mathbf{p}^l \cdot \left(\mathbf{g}^{l+\frac{1}{2}} - \mathbf{g}^{l-\frac{1}{2}}\right) \tag{79}$$

$$= \mathbf{p}^l \cdot \mathbf{P}^l + \frac{1}{\Delta x}\left(\frac{1}{2}\mathbf{p}^l \cdot \mathbf{g}^{l+\frac{1}{2}} + \frac{1}{2}\mathbf{p}^{l+1} \cdot \mathbf{g}^{l+\frac{1}{2}} + \frac{1}{2}\mathbf{p}^l \cdot \mathbf{g}^{l+\frac{1}{2}} - \frac{1}{2}\mathbf{p}^{l+1} \cdot \mathbf{g}^{l+\frac{1}{2}}\right)$$

$$-\frac{1}{\Delta x}\left(\frac{1}{2}\mathbf{p}^l \cdot \mathbf{g}^{l-\frac{1}{2}} + \frac{1}{2}\mathbf{p}^{l-1} \cdot \mathbf{g}^{l-\frac{1}{2}} + \frac{1}{2}\mathbf{p}^l \cdot \mathbf{g}^{l-\frac{1}{2}} - \frac{1}{2}\mathbf{p}^{l-1} \cdot \mathbf{g}^{l-\frac{1}{2}}\right)$$

$$= \mathbf{p}^l \cdot \mathbf{P}^l + \frac{1}{2}\frac{\mathbf{p}^{l+1} + \mathbf{p}^l}{\Delta x} \cdot \epsilon^{l+\frac{1}{2}} \frac{\Delta q^{l+\frac{1}{2}}}{\Delta x} - \frac{1}{2}\frac{\mathbf{p}^l + \mathbf{p}^{l-1}}{\Delta x} \cdot \epsilon^{l-\frac{1}{2}} \frac{\Delta q^{l-\frac{1}{2}}}{\Delta x} \quad - \frac{1}{2}\frac{\mathbf{p}^{l+1} - \mathbf{p}^l}{\Delta x} \cdot \epsilon^{l+\frac{1}{2}} \frac{\Delta q^{l+\frac{1}{2}}}{\Delta x} - \frac{1}{2}\frac{\mathbf{p}^l - \mathbf{p}^{l-1}}{\Delta x} \cdot \epsilon^{l-\frac{1}{2}} \frac{\Delta q^{l-\frac{1}{2}}}{\Delta x} \tag{80}$$

We know the identity

$$\int_{\mathbf{q}^l}^{\mathbf{q}^{l+1}} \mathbf{p} \cdot d\mathbf{q} = \int_{\mathbf{q}^l}^{\mathbf{q}^{l+1}} \partial_{\mathbf{q}} \mathcal{E} \cdot d\mathbf{q} = \mathcal{E}^{l+1} - \mathcal{E}^l = \Delta\mathcal{E}^{l+\frac{1}{2}} \tag{81}$$

We can now think of the term $\frac{1}{2}(p^{l+1} + p^l) \cdot \Delta\mathbf{q}^{l+\frac{1}{2}}$ as an approximation of the total energy density $\Delta\mathcal{E}^{l+\frac{1}{2}}$, where the path integral has been calculated using the trapezoidal rule. Thus, using the above two obtained equations, the energy flux, including the convective and diffusion terms, is

$$F_d^{l+\frac{1}{2}} = F_G^{l+\frac{1}{2}} - \frac{1}{2}(\mathbf{p}^{l+1} + \mathbf{p}^l) \cdot \epsilon^{l+\frac{1}{2}} \frac{\Delta q^{l+\frac{1}{2}}}{\Delta x} \approx F_G^{l+\frac{1}{2}} - \epsilon^{l+\frac{1}{2}} \frac{\Delta\mathcal{E}^{l+\frac{1}{2}}}{\Delta x} \tag{82}$$

10 Future Work

- Various dissipative terms, like numerical viscous terms, appropriate entropy production terms, relaxation terms, etc., will be analyzed and included in the system, thus creating a practical model.
- We will further take this system to multi-dimensional spaces.
- We will study its numerical convergence, and apply it to various numerical tests and problems in higher dimensions.

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