2017

Positivity-preserving finite volume methods for compressible Navier-Stokes equations

Heather Muchowski
Iowa State University

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Positivity-preserving finite volume methods for compressible Navier-Stokes equations

by

Heather Muchowski

A thesis submitted to the graduate faculty
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

Major: Applied Mathematics

Program of Study Committee:
Jue Yan, Major Professor
James Rossmanith
Paul Sacks

Iowa State University
Ames, Iowa
2017

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DEDICATION

I would like to dedicate this thesis to all of the people who provided guidance and support through this process. At the top of this list are my wonderful parents who have given me endless love and support through my whole mathematics career. Along with my parents, the life long friendships that I have made through this journey have kept me positive and pushed me to do my best. All of you have been there for me through the endless ups and downs of graduate school and I look forward to seeing what the future has in store for us.
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ACKNOWLEDGEMENTS

I would like to take this opportunity to express my thanks to those who helped me with various aspects of conducting research and the writing of this thesis. First and foremost, Dr. Jue Yan for her guidance, patience and support throughout my time at Iowa State University. Her insight, commitment, and patience were invaluable for my research and the writing of this thesis. I would also like to thank my committee members for their efforts and contributions to this work: Dr James Rossmanith and Dr. Paul Sacks.
ABSTRACT

In this thesis, we discuss first and second order finite volume methods to solve the one dimensional compressible Navier-Stokes equations. We prove the first order finite volume method preserves positivity for the density and pressure. We carry out a sequence of numerical tests including the famous Shock tube problem, extreme Riemann double rarefaction wave case, etc. For those cases with very low density, our scheme performed well and the density and pressure remain positive throughout the domain. We further consider to extend the positivity preserving discussion to second order finite volume methods.
CHAPTER 1. INTRODUCTION

Hyperbolic partial differential equations can be used to model a variety of physical phenomena such as traffic flow, fluid flow, air flow, and many others. In this thesis we study finite volume methods for the one dimensional compressible Navier-Stokes equations. Our goal is to obtain positive approximations to the density and pressure profiles.

To simulate a fast flying aircraft with compressible Navier-Stokes equations, it is common to encounter situations with low density and low pressure, which is close to a vacuum situation. For high order numerical method, it is very hard to obtain nonnegative approximations at all time levels. In this thesis, we consider first order and second order finite volume methods solving the compressible Navier-Stokes equations. We refer to the review articles [8] and [3] on numerical methods solving the compressible Navier-Stokes equations.

It is consistent to the physical meaning to obtain nonnegative approximations to the density and pressure. Furthermore maintaining nonnegative solutions is practically a very attractive property. For compressible flow, especially in the regime of high Mach number, the fluid velocity might be extremely high and the pressure might be very low. In such situations preserving the positivity of the density and pressure is very important. Negative pressure or density approximation will lead to an ill-posed system and practically cause the computation to blow up. Preserving the positivity can also be considered as a strong $L_{\infty}$ stability result for the numerical solutions. From stability point of view, it is very important to design numerical methods that can be proven to preserve positivity of the solution profiles.

In this thesis, we follow the framework of Zhang and Shu’s positivity preserving high order methods for the Euler equations [10] and [9]. Other studies, including [1], [2], [4], [6], [7] are on the high order discontinuous Galerkin methods to solve the compressible Navier-Stokes equations.
Under the conservation of mass, momentum and energy, mathematicians derive the compressible Navier-Stokes equations to model the air distribution around the wings of an aircraft. Let’s consider the following compressible Navier-Stokes equations for a one-dimensional setting,

\[
\begin{align*}
\rho_t + (\rho u)_x &= 0, \\
(\rho u)_t + (\rho u^2 + p)_x &= \frac{1}{Re} \left( \frac{4}{3} u_{xx} \right), \\
E_t + [u(E + p)]_x &= \frac{1}{Re} \left[ \left( \frac{2}{3} u^2 \right)_{xx} + \frac{1}{(\gamma - 1)Pr} (C^2)_{xx} \right],
\end{align*}
\]

with \(\rho, u,\) and \(E\) as the density, velocity, and total energy respectively and \(m = \rho u\) is the momentum \([9]\). We have parameter constants \(\gamma = 1.4\) for air and \(Pr = 0.7\) as the Prandtl number. We also have that \(C\) is the sound speed, related to pressure and density through the relation \(C = \sqrt{\gamma p/\rho}\). We have \(Re\) as the Reynolds number and the pressure function is given as \(p = (\gamma - 1)(E - \frac{1}{2}\rho u^2)\). Now we rewrite the system of equations (1.1) in vector format as,

\[
\begin{pmatrix}
\rho \\
\rho u \\
E
\end{pmatrix}_t + \begin{pmatrix}
\rho u \\
\rho u^2 + p \\
(E + p)u
\end{pmatrix}_x = \eta \frac{1}{Re} \begin{pmatrix}
0 \\
u \\
\frac{u^2}{2} + \frac{3C^2}{4(\gamma - 1)Pr}
\end{pmatrix}_{xx},
\]

with \(\mathbf{w} = (\rho, \rho u, E)^T = (\rho, m, E)^T\) as the conservative variables and \(\eta = \frac{4}{3}\). Equation (1.2) can be further simplified as the following,

\[
\mathbf{w}_t + F(\mathbf{w})_x = \frac{\eta}{Re} D(\mathbf{w})_{xx},
\]

where we define

\[
F(\mathbf{w}) = (f(\mathbf{w}), g(\mathbf{w}), h(\mathbf{w}))^T = (\rho u, \rho u^2 + p, u(E + p))^T
\]

and

\[
D(\mathbf{w}) = (D_1(\mathbf{w}), D_2(\mathbf{w}), D_3(\mathbf{w}))^T = \left( 0, u, \frac{1}{2} u^2 + \frac{3C^2}{4(\gamma - 1)Pr} \right)^T.
\]

Here, we call \(F(\mathbf{w})\) the inviscid term and \(D(\mathbf{w})\) the viscous term. To simplify the discussion, we consider periodic boundary conditions for most cases.

In this thesis we derive first and second order finite volume methods solving the compressible Navier-Stokes equations (1.2). We consider a piecewise constant numerical solution \(\mathbf{w}_j^n\) to
approximate the exact solution \( w(x, t) \) in the computational cell \( I_j \) at time level \( t_n \). Our goal is to prove that the piecewise constant numerical solution \( w^n_j \) and the corresponding pressure value \( p^n_j \) at all time levels stay in the admissible set \( G \), defined below,

\[
G = \{ w^n_j = (\rho^n_j, m^n_j, E^n_j)^T | \rho^n_j > 0 \text{ and } p^n_j = (\gamma - 1)\left(E^n_j - \frac{1}{2}(\rho^n_j (u^n_j)^2)\right) > 0, \forall j \forall n \}.
\]

The positivity preserving schemes refer to the numerical method where the states remain in the admissible set \( G \).

The organization of the thesis is the following. In Chapter 2 we derive the first order and second order finite volume methods for scalar hyperbolic conservation laws. In Chapter 3 we begin with the first order finite volume scheme solving the one dimensional compressible Navier-Stokes equations. Then, we carry out the positivity study of the density and pressure. We perform a sequence of numerical tests at the end of Chapter 3 that are consistent with the literature [9] to show the density and pressure remain non-negative in our simulations. In Chapter 4, we extend our studies to second order finite volume schemes for the compressible Navier-Stokes equations.
CHAPTER 2. FINITE VOLUME METHODS FOR CONSERVATION LAWS

In this chapter, we review the first order and second order finite volume methods for the scalar hyperbolic conservation laws. We have a conservative variable $u$, for example density, satisfying the following one dimensional nonlinear conservation law,

$$\frac{\partial}{\partial t} u(x, t) + \frac{\partial}{\partial x} f(u(x, t)) = 0,$$  (2.1)

associated with initial condition $u(x, t = 0) = u_0(x)$ and periodic boundary conditions. We refer to the books on numerical methods for nonlinear conservation laws [5].

To set up the finite volume scheme, we partition the spatial domain $[a, b]$ into $N$ cells. We denote the computational cell as $I_j = (x_{j-1/2}, x_{j+1/2})$ for $j = 1, ..., N$ with mesh size $\Delta x_j = x_{j+1/2} - x_{j-1/2}$. It can be seen that $x_{1/2} = a$ and $x_{N+1/2} = b$. Let’s denote $u_j^n$ to be the piecewise constant approximate solution to the exact solution $u(x, t)$ in cell $I_j$ and time level $t_n$.

2.1 First Order Finite Volume Scheme

Now let’s derive the first order finite volume scheme for (2.1). Integrating the equation over the computational cell $I_j$ we have,

$$\frac{\partial}{\partial t} \left( \int_{I_j} u(x, t) dx \right) + \int_{I_j} \frac{\partial}{\partial x} f(u) dx = 0.$$

Integrating the flux term out and dividing everything by the mesh size $\Delta x_j$, we obtain the following,

$$\frac{\partial}{\partial t} \left( \frac{1}{\Delta x_j} \int_{I_j} u(x, t) dx \right) + \frac{1}{\Delta x_j} \left( f(u(x_{j+1/2}, t)) - f(u(x_{j-1/2}, t)) \right) = 0.$$  (2.2)
This holds true for the exact solution and (2.2) is the starting point for designing finite volume methods. We introduce $u_j^n$ to be the piecewise constant approximation to the exact solution $u(x, t)$ over cell $I_j$ and time level $t_n$ given as

$$u_j^n \approx \frac{\int_{I_j} u(x, t_n) \, dx}{\Delta x_j}.$$

Discretizing in time using forward Euler and introducing the numerical flux $\hat{f}_{j\pm1/2}$ we obtain the following finite volume scheme,

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{1}{\Delta x_j} [\hat{f}_{j+1/2} - \hat{f}_{j-1/2}] = 0. \quad (2.3)$$

The numerical flux is not well defined at the cell interface $x_{j+1/2}$. We need to define the numerical flux $\hat{f}_{j\pm1/2}$ to approximate $f(u(x_{j\pm1/2}, t_n))$. We consider the Lax-Friedrichs type numerical flux given as,

$$\hat{f}_{j+1/2} = \hat{f}(u^-_{j+1/2}, u^+_{j+1/2}) = \frac{1}{2} [f(u^-_{j+1/2}) + f(u^+_{j+1/2}) - \alpha (u^+_{j+1/2} - u^-_{j+1/2})], \quad (2.4)$$

where $u_{j+1/2}^\pm$ are the approximations at $x_{j+1/2}$ from the given piecewise constant solutions. We have $\alpha = \max |f'(u(x, t))|$. With $\alpha$ evaluated over the whole domain we have the global Lax-Friedrich’s scheme and evaluated locally as the local Lax-Friedrich’s scheme. If we take the derivative of $\hat{f}$ with respect to $u_j^n$, we have $\frac{1}{2} \hat{f}'(u_j^n) + \frac{\alpha}{2}$ which should be greater than or equal to zero for monotonic stability and convergence. Then we have that $\alpha \geq -f'(u_j^n) \geq -\max |f'(u)|$. Thus, we can choose $\alpha = \max_{x \in [a, b]} |f'(u)|$ for all $u$.

The numerical flux must satisfy three conditions. First, it must be Lipschitz continuous in its arguments. Next, it must be consistent with $\hat{f}(u^*, u^*) = f(u^*)$ and lastly, it must be monotone increasing in the first variable and monotone decreasing in the second variable. These three conditions will guarantee the solution convergence to the viscosity solution.

Considering the first order approximation with $u^-_{j+1/2} = u_j^n$ and $u^+_{j+1/2} = u_{j+1}^n$, we have

$$\hat{f}_{j+1/2} = \hat{f}(u_j^n, u_{j+1}^n) = \frac{1}{2} [f(u_j^n) + f(u_{j+1}^n) - \alpha (u_{j+1}^n - u_j^n)]. \quad (2.5)$$

Rearranging the scheme formulation of (2.3), we obtain

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} [\hat{f}(u_j^n, u_{j+1}^n) - \hat{f}(u_{j-1}^n, u_j^n)]. \quad (2.6)$$
We call $a \frac{\Delta t}{\Delta x}$, where $a$ is the magnitude of velocity, the Courant-Friedrichs-Lewy (CFL) number. This CFL number must be chosen to be bounded by a small constant such as $\frac{1}{2}$ for low order approximations to guarantee stability. Now the first order finite volume scheme (2.6) for the scalar conservation law (2.1) is well defined.

### 2.2 Second Order Finite Volume Scheme

Now we consider a second order finite volume scheme solving the scalar conservation law (2.1). In this section we mainly discuss the second order finite volume scheme for space discretization. Later on we will incorporate high order Runge-Kutta methods, for example, to obtain a full second order scheme.

Recall the framework of the finite volume scheme (forward Euler in time) is as follows,

$$\frac{u_{j}^{n+1} - u_{j}^{n}}{\Delta t} + \frac{1}{\Delta x_{j}} [\hat{f}_{j+1/2} - \hat{f}_{j-1/2}] = 0.$$  

We consider a second order approximation of $u_{j+1/2}^{\pm}$ and $u_{j-1/2}^{\pm}$ in (2.4). Let’s focus on the cell interface $x_{j+1/2}$. Generally $u_{j+1/2}^{\pm}$ should be evaluated from high order reconstruction polynomials. For the second order case, we need to reconstruct two linear polynomials $P_{1}^{+}(x)$ and $P_{1}^{-}(x)$ using the given piecewise constant solution $u_{j}^{n}$, $u_{j+1}^{n}$ and $u_{j-1}^{n}$. To be more specific, $P_{1}^{-}$ is reconstructed with the fact that its average in cell $I_{j}$ and $I_{j-1}$ is set to $u_{j}^{n}$ and $u_{j-1}^{n}$. In a word, to determine $P_{1}^{-}(x) = ax + b$ where $a$ and $b$ are some constants, we then enforce

$$\frac{1}{\Delta x} \int_{I_{j}} P_{1}^{-}(x) \, dx = u_{j}^{n},$$  

$$\frac{1}{\Delta x} \int_{I_{j-1}} P_{1}^{-}(x) \, dx = u_{j-1}^{n}.$$  

We can solve this system of equations to obtain constants $a$ and $b$. Note that we have
uniform partition. For simplicity, let $x_{j+1/2} = x_2$, $x_{j-1/2} = x_1$ and $x_{j-3/2} = x_0$. Then,

$$
\frac{1}{\Delta x} \int_{x_1}^{x_2} (ax + b) \, dx = u_j^n
$$

Using integration by parts,

$$
a \frac{x^2}{2} + bx \bigg|_{x_1}^{x_2} = \Delta x u_j^n
$$

$$
\frac{a}{2} (x_2^2 - x_1^2) + b(x_2 - x_1) = \Delta x u_j^n
$$

$$
\frac{a}{2} (x_2 - x_1)(x_2 + x_1) + b(x_2 - x_1) = \Delta x u_j^n
$$

$$
\frac{a}{2} (x_2 + x_1) \Delta x + b \Delta x = \Delta x u_j^n
$$

This gives us

$$
a \frac{2}{2}(x_2 + x_1) + b = u_j^n. \tag{2.7}
$$

Solving the second equation similarly to above yields

$$
a \frac{2}{2}(x_1 + x_0) + b = u_{j-1}^n. \tag{2.8}
$$

We subtract (2.8) from (2.7) to obtain

$$
a = \frac{u_j^n - u_{j-1}^n}{\Delta x}
$$

and

$$
b = u_j^n - \frac{(u_j^n - u_{j-1}^n)}{2\Delta x}(x_2 + x_1).
$$

This gives polynomial $P_1^-(x)$ to be

$$
P_1^-(x) = \left( \frac{u_j^n - u_{j-1}^n}{\Delta x} \right) x + u_j^n - \frac{(u_j^n - u_{j-1}^n)}{2\Delta x}(x_2 + x_1).
$$

Now we evaluate $P_1^-(x)$ at $x_{j+1/2}$ as an approximation to $u_{j+1/2}^-$, we have,

$$
u_{j+1/2}^- = u_j^n + \frac{1}{2}(u_j^n - u_{j-1}^n). \tag{2.9}
$$

or

$$
u_{j+1/2}^- = \frac{1}{2}(3u_j^n - u_{j-1}^n).
$$

From approximation theory we have $P_1(x) \approx u(x, t_n) + O(\Delta x^2)$. 
Now we consider to reconstruct $P_1^+(x)$ from the given cell average $u^n_j$, $u^n_{j+1}$. Let $P_1^+(x) = cx + d$ where $c$ and $d$ are some constants. We can then enforce,

$$\frac{1}{\Delta x} \int_{I_j} P_1^-(x) dx = u^n_j,$$
$$\frac{1}{\Delta x} \int_{I_{j+1}} P_1^-(x) dx = u^n_{j+1}.$$ 

Following the process above to obtain value for $c$ and $d$, we obtain

$$c = \frac{u^n_{j+1} - u^n_j}{\Delta x}$$

and

$$d = u^n_j - \frac{(u^n_{j+1} - u^n_j)}{2\Delta x}(x_2 + x_1).$$

Combining these we have the reconstruction polynomial,

$$P_1^+(x) = \left(\frac{u^n_{j+1} - u^n_j}{\Delta x}\right)x + u^n_j - \frac{(u^n_{j+1} - u^n_j)}{2\Delta x}(x_2 + x_1).$$

Evaluating at $x_{j+1/2} = x_2$, we obtain the approximation at $u^+_{j+1/2}$,

$$u^+_{j+1/2} = u^n_j + \frac{1}{2}(u^n_{j+1} - u^n_j) \quad (2.10)$$

or

$$u^+_{j+1/2} = \frac{1}{2}(u^n_{j+1} + u^n_j).$$

To finish up the second order finite volume scheme, we only need to plug in the second order approximation $u^-_{j+1/2}$ from (2.9) and $u^+_{j+1/2}$ from (2.10) into the Lax-Friedrichs flux numerical expression (2.4),

$$\hat{f}(u^-_{j+1/2}, u^+_{j+1/2}) = \frac{1}{2} (f(u^-_{j+1/2}) + f(u^+_{j+1/2}) - \alpha (u^+_{j+1/2} - u^-_{j+1/2})).$$

Thus, we finish out the discussion for the second order finite volume method for the scalar conservation law (2.1).
CHAPTER 3. FIRST ORDER FINITE VOLUME SCHEME FOR COMPRESSIBLE NAVIER-STOKES EQUATIONS

In this chapter we study finite volume methods for the one dimensional compressible Navier-Stokes equations given as,

\[
\begin{align*}
\rho_t + (\rho u)_x &= 0, \\
(\rho u)_t + (\rho u^2 + p)_x &= \frac{1}{Re} \left( \frac{4}{3} u_{xx} \right), \\
E_t + [u(E + p)]_x &= \frac{1}{Re} \left[ \left( \frac{2}{3} u^2 \right)_{xx} + \frac{1}{(\gamma - 1)Pr} (C^2)^{xx} \right].
\end{align*}
\tag{3.1}
\]

where \(w = (\rho, \rho u, E)^T = (\rho, m, E)^T\) are the conservative variables with \(\rho, u,\) and \(E\) as the density, velocity, and total energy, respectively and \(m = \rho u\) is the momentum \[9\]. We have parameter constraints \(\gamma = 1.4\) for air and \(Pr = 0.7\) is the Prandtl number. We also have that \(C\) is the sound speed, related to pressure and density through relation \(C = \sqrt{\gamma p/\rho}\). Then, \(Re\) is the Reynolds number and the pressure function given as \(p = (\gamma - 1)(E - \frac{1}{2} \rho u^2)\). We can rewrite the system of equations (3.1) as

\[
\begin{pmatrix}
\rho \\
\rho u \\
E
\end{pmatrix}_t + \begin{pmatrix}
\rho u \\
\rho u^2 + p \\
(E + p)u
\end{pmatrix}_x = \frac{\eta}{Re} \begin{pmatrix}
0 \\
u \\
u^2 + \frac{3C^2}{4(\gamma - 1)Pr}
\end{pmatrix}_{xx},
\]

where \(\eta = \frac{4}{3}\).

We can simplify the above system of equations even further as,

\[
\begin{align*}
\mathbf{w}_t + F(\mathbf{w})_x &= \frac{\eta}{Re} D(\mathbf{w})_{xx}, \\
\end{align*}
\tag{3.2}
\]

where we define

\[
F(\mathbf{w}) = (f(\mathbf{w}), g(\mathbf{w}), h(\mathbf{w}))^T = (\rho u, \rho u^2 + p, u(E + p))^T
\tag{3.3}
\]
and
\[ D(w) = (D_1(w), D_2(w), D_3(w))^T = \left( 0, u, \frac{1}{2} u^2 + \frac{3C^2}{4(\gamma - 1)Pr} \right)^T. \] (3.4)

Here, we call \( F(w) \) the inviscid term and \( D(w) \) the viscous term. The initial condition is given as \( w(x, t = 0) = w_0(x) \) and we consider periodic boundary conditions.

To set up the finite volume scheme, we partition the spatial domain \([a, b]\) into \( N \) cells denoted as \( I_j = (x_{j-1/2}, x_{j+1/2}) \) for \( j = 1, ..., N \) and mesh size \( \Delta x_j = x_{j+1/2} - x_{j-1/2} \). We have that \( x_{1/2} = a \) and \( x_{N+1/2} = b \). We now introduce new notation. Let \( w_j^n = (\rho_j^n, m_j^n, E_j^n) \) be the approximated solution to \( w \) at time level \( t_n \) and inside cell \( I_j \) and define,

\[ \rho_j^n \approx \int_{I_j} \rho(x, t_n) dx / \Delta x_j, \]
\[ m_j^n \approx \int_{I_j} m(x, t_n) dx / \Delta x_j, \]
\[ E_j^n \approx \int_{I_j} E(x, t_n) dx / \Delta x_j. \]

The pressure function \( p_j^n \) can be directly evaluated from,
\[ p_j^n = (\gamma - 1) \left( E_j^n - \frac{(m_j^n)^2}{2\rho_j^n} \right). \]

Our goal for the chapter is to prove at all time levels the density and the pressure approximations remain positive. In section 3.1 we study the first order finite volume scheme. In section 3.2 we study the positivity of the density and in section 3.3 we study the positivity of the pressure. In section 3.4 we carry out numerical tests.

### 3.1 First Order Finite Volume Scheme

We first write out the first order finite volume scheme of (1.2) for the compressible Navier-Stokes equation. Now we must discretize in space and time. We consider the forward Euler discretization in time and first order finite volume method in space. Here, we apply the first order finite volume scheme for scalar conservation laws (2.6) to the compressible Navier-Stokes equations (1.2) to obtain,
\[ w_j^{n+1} = w_j^n - \frac{\Delta t}{\Delta x} \left[ \hat{F}(w_j^n, w_{j+1}^n) - \hat{F}(w_{j-1}^n, w_j^n) \right]. \]
Refer to (2.6) for the definition of the numerical flux $\hat{f}_{j\pm 1/2}$. We can write out $\hat{F}$ as

$$\hat{F}(w^n_{j}, w^n_{j+1}) = \frac{1}{2}[F(w^n_{j}) + F(w^n_{j+1}) - \alpha(w_{j+1} - w_{j})],$$

$$\hat{F}(w^n_{j-1}, w^n_{j}) = \frac{1}{2}[F(w^n_{j-1}) + F(w^n_{j}) - \alpha(w_{j} - w_{j-1})].$$

Here, $\alpha$ is the largest eigenvalue of the $3 \times 3$ Jacobian matrix. Thus, $\alpha = ||u|| + C||_{\infty}$, where $C = \sqrt{\frac{\gamma p}{\rho}}$, also known as the sound speed.

Let’s consider the discretization of the diffusion term. We consider the following simple diffusion equation with finite volume method,

$$u_t - d(u)_{xx} = 0.$$  

We derive the scheme by integrating the diffusion term over cell $I_j$,

$$\frac{1}{\Delta x_j} \int_{I_j} d(u)_{xx} dx = \frac{d(u)x(x_{j+1/2}) - d(u)x(x_{j-1/2})}{\Delta x_j}.$$  

Then we apply the one sided finite volume scheme to approximate the derivative at $x_{j+1/2}$ and $x_{j-1/2}$ defined as

$$d(u)x|_{x_{j+1/2}} \approx \frac{d(u_{j+1}) - d(u_{j})}{\Delta x},$$

$$d(u)x|_{x_{j-1/2}} \approx \frac{d(u_{j}) - d(u_{j-1})}{\Delta x}.$$  

We can then use these to build up the second order finite volume scheme solving the previous diffusion equation. Thus,

$$\frac{1}{\Delta x} \int_{I_j} d(u)_{xx} dx \approx \frac{d(u_{j+1}) - 2d(u_{j}) + d(u_{j-1})}{\Delta x^2}.$$  \hspace{1cm} (3.5)$$

Now we apply (3.5) to the viscous term of the compressible Navier-Stokes equations given in (1.2) to finish up the discretization in space. Combining forward Euler discretization in time and the first order finite volume scheme for the inviscid term detailed above, finally we obtain the full scheme as follows,

$$w^{n+1}_{j} = w^n_{j} - \frac{\Delta t}{\Delta x} \left( \hat{F}(w^n_{j}, w^n_{j+1}) - \hat{F}(w^n_{j-1}, w^n_{j}) \right) + \frac{\Delta t}{\Delta x^2} \eta \frac{\Delta t}{Re} \left( D(w^n_{j+1}) - 2D(w^n_{j}) + D(w^n_{j-1}) \right).$$  \hspace{1cm} (3.6)$$
Algorithm 1:

1) We set up the mesh $I_j$ and carry out initialization of the finite volume numerical solution. Then we define constants $\gamma$, $Re$, and $Pr$. We initialize initial conditions $(\rho_j^0, m_j^0, E_j^0)$ at time level $t_0$.

2) While $t_{\text{current}} < T_{\text{final}}$, calculate $p_j^n$, $C_j^n$ and compute $\alpha$, where pressure can be directly approximated by,

$$p_j^n = (\gamma - 1)(E_j^n - \frac{1}{2} (m_j^n)^2).$$

In a separate for loop, we can compute the values for $\rho$, $m$, and $E$ at the next time level given as,

$$\rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{\Delta x} \left[ f(w_j^n, w_{j+1}^n) - f(w_{j-1}^n, w_j^n) \right] + \frac{\Delta t}{\Delta x^2} \frac{\eta}{Re} \left[ D_1(w_{j+1}^n) - 2D_1(w_j^n) + D_1(w_{j-1}^n) \right]$$

$$m_j^{n+1} = m_j^n - \frac{\Delta t}{\Delta x} \left[ g(w_j^n, w_{j+1}^n) - g(w_{j-1}^n, w_j^n) \right] + \frac{\Delta t}{\Delta x^2} \frac{\eta}{Re} \left[ D_2(w_{j+1}^n) - 2D_2(w_j^n) + D_2(w_{j-1}^n) \right]$$

$$E_j^{n+1} = E_j^n - \frac{\Delta t}{\Delta x} \left[ h(w_j^n, w_{j+1}^n) - h(w_{j-1}^n, w_j^n) \right] + \frac{\Delta t}{\Delta x^2} \frac{\eta}{Re} \left[ D_3(w_{j+1}^n) - 2D_3(w_j^n) + D_3(w_{j-1}^n) \right]$$

where

$$f(w_j^n, w_{j+1}^n) = \frac{1}{2} (m_j^n + m_{j+1}^n - \alpha(m_{j+1}^n - m_j^n))$$

$$g(w_j^n, w_{j+1}^n) = \frac{1}{2} \left( \frac{(m_j^n)^2}{\rho_j^n} + (\gamma - 1)(E_j^n - \frac{1}{2} (m_j^n)^2) + \frac{(m_{j+1}^n)^2}{\rho_{j+1}^n} \right)$$

$$+ (\gamma - 1)(E_{j+1}^n - \frac{1}{2} (m_{j+1}^n)^2) - \alpha(m_{j+1}^n - m_j^n))$$

$$h(w_j^n, w_{j+1}^n) = \frac{1}{2} \left( \frac{m_j^n}{\rho_j^n} (E_j^n + (\gamma - 1)(E_j^n - \frac{1}{2} (m_j^n)^2)) + \frac{m_{j+1}^n}{\rho_{j+1}^n} (E_{j+1}^n + (\gamma - 1)(E_{j+1}^n - \frac{1}{2} (m_{j+1}^n)^2)) \right)$$

$$+ (\gamma - 1)(E_{j+1}^n - \frac{1}{2} (m_{j+1}^n)^2) - \alpha(E_{j+1}^n - E_j^n),$$

and

$$D_1(w) = 0,$$

$$D_2(w) = \frac{m}{\rho}$$

$$D_3(w) = \frac{m^2}{2 \rho^2} + \frac{3C^2}{4(\gamma - 1)Pr}.$$
The focus of this thesis is to study the positivity of the density and pressure approximations. We are going to prove the numerical approximation of the density \( \rho_j^n \) and the pressure value \( p_j^n \) remain in the admissible set \( G \),

\[
G = \{ w_j^n = (\rho_j^n, m_j^n, E_j^n)^T | \rho_j^n > 0 \text{ and } p_j^n = (\gamma - 1)(E_j^n - \frac{1}{2}\rho_j^n(u_j^n)^2) > 0, \forall j, \forall n \}
\]

for all time levels.

One important property is that the pressure function \( p(w) = (\gamma - 1)(E - \frac{m_2}{2\rho}) \) is a concave function in terms of the conservative variables if \( \rho > 0 \). Consider two states \( w_1 \) with \( \rho_1 > 0 \) and \( w_2 \) with \( \rho_2 > 0 \). Then, convexity implies that

\[
p(sw_1 + (1 - s)w_2) \geq sp(w_1) + (1 - s)p(w_2), \quad 0 \leq s \leq 1. \quad (3.7)
\]

The idea is to prove that at the next time level, \( t_{n+1} \), the state \( w_j^{n+1} \) can be written out as a convex combination of the solution states at the previous time level, \( w_j^n \). Then we apply the property (3.7) to show that \( p_j^{n+1} = p(w_j^{n+1}) > 0 \).

Let’s organize the right hand side of (3.6) and show that \( w_j^{n+1} \) can be written out as a convex combination of states at the previous time level. Then we will show one by one that the pressure value at each state in this combination is positive. Now lets plug in the numerical flux \( \hat{F}(\cdot, \cdot) \) into the scheme (3.6) and reorganize into states to obtain the following,

\[
\begin{align*}
\rho_j^{n+1} &= \left(1 - \alpha \frac{\Delta t}{\Delta x}\right) \rho_j^n + \alpha \frac{\Delta t}{2\Delta x} \left(\rho_j^{n+1} - \frac{f(\rho_j^{n+1})}{\alpha}\right) + \alpha \frac{\Delta t}{2\Delta x} \left(\rho_j^{n-1} + \frac{f(\rho_j^{n-1})}{\alpha}\right) \\
&\quad + \frac{\Delta t}{Re\Delta x^2} D(w_j^{n+1}) + \frac{\Delta t}{Re\Delta x^2} D(w_j^{n-1}) + \left(1 - \frac{2\Delta t}{Re\Delta x^2} D(w_j^n)\right) \\
&\quad = \text{Inviscid term} + \text{Viscous term}. \quad (3.8)
\end{align*}
\]

### 3.2 Positivity of Density

In this section we prove that the density is positive at all time levels. We use the convexity argument from (3.8) with just density involved. Take note that since density is the first entry of vector \( w \) with \( D_1(w) = 0 \), we have no contribution of the viscous term. Then the first component of (3.8) is the following,

\[
\rho_j^{n+1} = \left(1 - \alpha \frac{\Delta t}{\Delta x}\right) \rho_j^n + \alpha \frac{\Delta t}{2\Delta x} \left(\rho_j^{n+1} - \frac{f(\rho_j^{n+1})}{\alpha}\right) + \alpha \frac{\Delta t}{2\Delta x} \left(\rho_j^{n-1} + \frac{f(\rho_j^{n-1})}{\alpha}\right). \quad (3.9)
\]
With proper CFL restrictions, \( \alpha \frac{\Delta t}{\Delta x} < 1 \), we have that the first term of (3.9) is positive. We can see that the coefficient of the second term of (3.9) is positive if \( \rho - \frac{\rho u}{\alpha} > 0 \) or that \( 1 > \frac{u}{\alpha} \).

Recall that \( \alpha = \| |u| + C| \|_\infty \), where \( C = \sqrt{\gamma \rho} \), so obviously we have \( 1 > |\frac{u}{\alpha}| \). Then we know that \( -1 < \frac{u}{\alpha} < 1 \), so the previous inequality holds and \( \rho - \frac{f(\rho)}{\alpha} > 0 \). Similarly for the third term, \( \rho + \frac{f(\rho)}{\alpha} > 0 \) if \( \rho + \frac{\rho u}{\alpha} > 0 \) or if \( -1 < \frac{u}{\alpha} \). Thus, the third term of (3.9) is also positive.

Therefore, we have just shown that density can be maintained positive at all time levels.

### 3.3 Positivity of Pressure

Recall the convex combination of states from (3.8),

\[
\mathbf{w}^{n+1}_j = \left( \frac{1}{2} - \alpha \frac{\Delta t}{\Delta x} \right) \mathbf{w}^n_j + \frac{\alpha \Delta t}{2 \Delta x} \left( \mathbf{w}^n_{j+1} - \frac{F(\mathbf{w}^n_{j+1})}{\alpha} \right) + \frac{\alpha \Delta t}{2 \Delta x} \left( \mathbf{w}^n_{j-1} + \frac{F(\mathbf{w}^n_{j-1})}{\alpha} \right) \\
+ \frac{\Delta t}{Re \Delta x^2} D(\mathbf{w}^n_{j+1}) + \frac{\Delta t}{Re \Delta x^2} D(\mathbf{w}^n_{j-1}) + \left( \frac{1}{2} \mathbf{w}^n_j - \frac{2 \Delta t}{Re \Delta x^2} D(\mathbf{w}^n_j) \right).
\]

With suitable CFL restrictions on the time step size, \( \alpha \frac{\Delta t}{\Delta x} < 1 \), we see the weights of the six states in (3.8) are all positive. Now we must show that the corresponding pressure values of each state is positive. We separate the discussion into the first three inviscid terms and the last three viscous terms.

#### 3.3.1 Discussion on Inviscid terms

Suppose \( \mathbf{w}^n_j \) for all \( j \) stays in the admissible set \( G \) such that the pressure value \( p(\mathbf{w}^n_j) \) for all \( j \) is also positive. The first term pressure value \( p(\left( \frac{1}{2} - \alpha \frac{\Delta t}{\Delta x} \right) \mathbf{w}^n_j) = \left( \frac{1}{2} - \alpha \frac{\Delta t}{\Delta x} \right) p(\mathbf{w}^n_j) \) is positive under the CFL restriction \( \frac{1}{2 \alpha} > \frac{\Delta t}{\Delta x} \) since we have \( p(\mathbf{w}^n_j) > 0 \). We only need to show the pressure value of the second and third states remain positive. Dropping the sub and super scripts, we now show that \( p(\mathbf{w} - \frac{F(\mathbf{w})}{\alpha}) > 0 \) where \( \mathbf{w} = (\rho, m, E)^T \) and \( F(\mathbf{w}) = (m, \rho u^2 + p, Eu + pu)^T \).
Denote \( u = \frac{m}{\rho} \). Then we have,

\[
p \left( \frac{w - F(w)}{\alpha} \right) = p \left( \left( \rho - \frac{m}{\alpha}, m - \frac{mu + p}{\alpha}, E - \frac{(E + p)u}{\alpha} \right)^T \right)
\]

\[
= (\gamma - 1) \left( E - \frac{(E + p)u}{\alpha} - \frac{(m - \frac{mu + p}{2}(\rho - \frac{m}{\alpha}))}{2\rho(1 - \frac{m}{\alpha})} \right)
\]

\[
= (\gamma - 1) \left( E - \frac{(E + p)u}{\alpha} - \frac{((1 - \frac{u}{\alpha})m - \frac{p}{\alpha})(1 - \frac{u}{\alpha})m - \frac{p}{\alpha})}{2\rho(1 - \frac{m}{\alpha})} \right)
\]

\[
= (\gamma - 1) \left( (1 - \frac{u}{\alpha}) E - \frac{u}{\alpha}p - \left( \frac{1 - \frac{u}{\alpha}}{2\rho} - \frac{mp}{\rho\alpha} + \frac{p^2}{2\alpha^2\rho(1 - \frac{u}{\alpha})} \right) \right).
\]

Recall that \( u = \frac{m}{\rho} \). Then we have,

\[
p \left( \frac{w - F(w)}{\alpha} \right) = (\gamma - 1) \left( (1 - \frac{u}{\alpha}) E - \frac{u}{\alpha}p - \left( \frac{1 - \frac{u}{\alpha}}{2\rho} + \frac{up}{\alpha} - \frac{p^2}{2\alpha^2\rho(1 - \frac{u}{\alpha})} \right) \right)
\]

\[
= (\gamma - 1) \left( (1 - \frac{u}{\alpha}) E - \frac{u}{\alpha}p - \left( \frac{1 - \frac{u}{\alpha}}{2\rho} - \frac{mp}{\rho\alpha} + \frac{p^2}{2\alpha^2\rho(1 - \frac{u}{\alpha})} \right) \right)
\]

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

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

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

Note that the pressure value in the above equations is evaluated in cell \( I_j \) at time level \( t_n \).

Given that \( \alpha = ||u|| + C \| \infty \), where \( C = \sqrt{\gamma p}/\rho \), we have that \( \frac{u}{\alpha} < 1 \). Therefore, \( (1 - \frac{u}{\alpha}) > 0 \).

Thus, to show \( p(w - \frac{F(w)}{\alpha}) > 0 \) we must show that \( (1 - \frac{p\gamma(\alpha - u)}{2\rho(\alpha - u)}) > 0 \). Then, we have

\[
1 > \frac{p\gamma(\alpha - u)}{2\rho(\alpha - u)}
\]

\[
1 > \frac{\gamma p\gamma(\alpha - u)}{2\rho\gamma(\alpha - u)^2}
\]

\[
1 > \frac{C^2(\gamma - 1)}{2\gamma(\alpha - u)^2}
\]

Then, we can manipulate the equation,

\[
\Rightarrow 1 < \frac{2(\alpha - u)^2\gamma}{(\gamma - 1)C^2}
\]

\[
\Rightarrow C^2 < \frac{2(\alpha - u)^2\gamma}{(\gamma - 1)}
\]

\[
\Rightarrow C < \sqrt{2\gamma/(\gamma - 1)(\alpha - u)}.
\]
Thus, we have that $(1 - \frac{p(\gamma-1)}{2\rho(\alpha-u)^2}) > 0$ if $C = \sqrt{\gamma p/\rho} < \sqrt{2\gamma/(\gamma-1)(\alpha-u)}$, which is trivially true when $\gamma = 1.4$. Thus, we have that the pressure at this state is positive.

Now we can follow a similar process to show that the pressure at state $w_{j-1}^n + \frac{F(w_{j-1}^n)}{\alpha}$ is also positive. We have,

$$p(w + \frac{F(w)}{\alpha}) = p \left( \left( \rho + \frac{m}{\alpha}, m + \frac{mu + p}{\alpha}, E + \frac{(E + p)u}{\alpha} \right)^T \right)$$

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

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

As we showed above, $|\frac{u}{\alpha}| < 1$, so we have that $(1 + \frac{u}{\alpha}) > 0$ and also that $(1 - \frac{p(\gamma-1)}{2\rho(\alpha+u)^2}) > 0$. Thus the pressure at state $w_{j-1}^n + \frac{F(w_{j-1}^n)}{\alpha}$ is positive.

### 3.3.2 Discussion on Viscous Terms

Now let's consider the three viscous terms and denote $\mu = 2 \frac{\Delta t}{\Delta x^2} \frac{\eta}{Re}$ for convenience and drop the superscript $n$ on the right hand side. Then, we can write $w$ as

$$w_{i+1}^n = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} + \mu \begin{bmatrix} 0 \\ u \\ \frac{u^2}{2} + \frac{3C^2}{4(\gamma-1)Pr} \end{bmatrix}_{i-1} - 2 \begin{bmatrix} 0 \\ u \\ \frac{u^2}{2} + \frac{3C^2}{4(\gamma-1)Pr} \end{bmatrix}_i + \begin{bmatrix} 0 \\ u \\ \frac{u^2}{2} + \frac{3C^2}{4(\gamma-1)Pr} \end{bmatrix}_{i+1}$$

We notice that there is a zero in the first row of the right hand side. This physically does not make sense as this would be a vacuum state, so we change those to ones. This is mathematically equivalent because it still turns out to be zero after the addition of the first component. Equivalently we have,

$$w_{i+1}^n = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} + \mu \begin{bmatrix} 1 \\ u \\ \frac{u^2}{2} + \frac{3C^2}{4(\gamma-1)Pr} \end{bmatrix}_{i-1} - 2 \begin{bmatrix} 1 \\ u \\ \frac{u^2}{2} + \frac{3C^2}{4(\gamma-1)Pr} \end{bmatrix}_i + \begin{bmatrix} 1 \\ u \\ \frac{u^2}{2} + \frac{3C^2}{4(\gamma-1)Pr} \end{bmatrix}_{i+1}$$

$$= \frac{\mu}{2} \begin{pmatrix} 1 \\ u \\ \frac{u^2}{2} + \frac{3C^2}{4(\gamma-1)Pr} \end{bmatrix}_{i-1} + \mu \begin{pmatrix} 1 \\ u \\ \frac{u^2}{2} + \frac{3C^2}{4(\gamma-1)Pr} \end{bmatrix}_{i+1} + \begin{pmatrix} \rho \\ \rho u - \mu \\ \frac{u^2}{2} + \frac{3C^2}{4(\gamma-1)Pr} \end{pmatrix}_i$$
Let’s define the function

\[ \mathcal{X}(w) = \rho E - \frac{1}{2} |\rho u|^2. \]

We can see that a vector \( w \) stays in the admissible set \( G \) is equivalent to its first component and \( \mathcal{X}(w) \) being positive. At time level \( t_n \) we have \( w^n \in G \). Let’s consider the first state in the above right hand side combination \((1, u, \frac{u^2}{2} + \frac{C^2}{(\gamma - 1)Pr\eta})^T\). The first component is obviously positive, then we must check that \( \mathcal{X}((1, u, \frac{u^2}{2} + \frac{C^2}{(\gamma - 1)Pr\eta}))^T > 0 \). We have

\[
\mathcal{X}\left(\begin{pmatrix}
1 \\
u \\
\frac{u^2}{2} + \frac{C^2}{(\gamma - 1)Pr\eta}
\end{pmatrix}\right) = \frac{u^2}{2} + \frac{C^2}{(\gamma - 1)Pr\eta} - \frac{1}{2} |u|^2 = \frac{C^2}{(\gamma - 1)Pr\eta} > 0.
\]

Thus, we just proved that the state \((1, u, \frac{u^2}{2} + \frac{C^2}{(\gamma - 1)Pr\eta})^T\) belongs to the admissible set \( G \). Now consider the last state and denote,

\[
V = \begin{pmatrix}
\rho \\
\rho u \\
E
\end{pmatrix} - \mu \begin{pmatrix}
1 \\
u \\
\frac{u^2}{2} + \frac{C^2}{(\gamma - 1)Pr\eta}
\end{pmatrix}.
\]

Notice that we have \( w = \begin{pmatrix}
\rho \\
\rho u \\
E
\end{pmatrix} \) at cell \( I_j \) and time level \( t_n \) belongs to the admissible set \( G \).

Notice that the first component of \( V \) is \( \rho - \mu \). We know that this is greater than or equal to zero if the following condition is satisfied for the previous argument to hold true,

\[
\frac{2 \Delta t \eta}{\Delta x Re} \leq \min_i \rho_i.
\]
Then, we have

\[ X(V) = (\rho - \mu) \left( E - \mu \left( \frac{u^2}{2} + \frac{C^2}{(\gamma - 1)Pr\eta} \right) \right) - \frac{1}{2} (\rho u - \mu u)^2 \]

\[ = \rho E - \mu \rho \left( \frac{u^2}{2} + \frac{C^2}{(\gamma - 1)Pr\eta} \right) - \mu E + \mu^2 \left( \frac{u^2}{2} + \frac{C^2}{(\gamma - 1)Pr\eta} \right) - \frac{1}{2} \rho^2 u^2 - \frac{1}{2} \mu^2 u^2 + \rho \mu u^2 \]

\[ = (\rho - \mu)(E - \frac{1}{2} \rho u^2) - \frac{\rho \mu C^2}{(\gamma - 1)Pr\eta} + \frac{C^2\mu^2}{(\gamma - 1)Pr\eta} \]

\[ = (\rho - \mu) \frac{p}{\gamma - 1} - \frac{\rho \mu \gamma p}{\rho(\gamma - 1)Pr\eta} + \frac{\gamma p \mu^2}{\rho(\gamma - 1)Pr\eta} \]

\[ = \frac{p}{\gamma - 1} \left[ (\mu - \rho) \left( \frac{\mu \gamma}{\rho Pr\eta} - 1 \right) \right]. \]

Since we have that \( \rho - \mu \geq 0 \) with the above condition, we have that \( X(V) \geq 0 \) if \( \frac{\mu \gamma}{\rho Pr\eta} - 1 \leq 0 \), or \( \frac{\mu \gamma}{Pr\eta} \leq \rho_i \). Thus, we need the following condition to be satisfied,

\[ 2 \Delta t \Delta x^2 \frac{\gamma}{Pr Re} \leq \min_i \rho_i. \]

Thus, we have proved that if \( w_i^0 \in G \) for all \( i \) then \( w_i^{n+1} \in G \) under the CFL constraint,

\[ \Delta t \leq \frac{1}{2} \min \left\{ \frac{1}{\eta}, \frac{Pr}{\gamma} \right\} \min_i \rho_i Re \Delta x^2. \]

**Theorem** For the first order finite volume scheme (3.8) solving (1.2), if \( w_i^n \) is in the admissible set \( G \) for all \( i \), then \( w_i^{n+1} \) is in \( G \) under the CFL constraint

\[ \frac{\Delta t}{\Delta x} \leq \min \left( \frac{1}{2} \min \left\{ \frac{1}{\eta}, \frac{Pr}{\gamma} \right\} \min_i \rho_i Re \Delta x, \frac{1}{2\alpha} \right). \]

### 3.4 Numerical Tests

We carry out a sequence of numerical tests for the compressible Navier-Stokes equations (1.2) with various initial conditions. We tested the famous Lax shock tube problem, extreme Riemann problem, etc. For those close to a vacuum situation with very low density and pressure, we see the first order finite volume scheme performs well. Shocks, rarefaction waves, contact discontinuities are all captured well.

**Example 1** (Accuracy Test) We test the accuracy of the first order finite volume scheme for the compressible Navier-Stokes equations with \( Re = 100 \). We use the initial data given as
\[ \rho = 1, \ u = 0 \text{ and } E = \frac{12}{\gamma - 1} + \frac{1}{2} \exp(-4 \cos^2 x^2). \] Boundary conditions are periodic on the interval 
[0, 2\pi]. The reference solution was generated by running the scheme with 10,000 cells. The \( L^\infty \) error between the two schemes is given in the following table.

<table>
<thead>
<tr>
<th>Table 3.1 Accuracy Table for Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N = 10 )</td>
</tr>
<tr>
<td>----------------</td>
</tr>
<tr>
<td>( L^\infty ) error</td>
</tr>
<tr>
<td>Ratio</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 3.2 Accuracy Table for Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N = 10 )</td>
</tr>
<tr>
<td>----------------</td>
</tr>
<tr>
<td>( L^\infty ) error</td>
</tr>
<tr>
<td>Ratio</td>
</tr>
</tbody>
</table>

For a first order method we should obtain the ratio to be about 2. We see in our results the ratio is lower than two so there must be some sort of bug in the code.

**Example 2** (The Lax shock tube problem.) We test the first order finite volume scheme for the following Lax shock tube problem. The initial conditions are given as

\[
\begin{pmatrix}
\rho \\
m \\
E
\end{pmatrix}
= \begin{pmatrix} 1 \\ 0 \\ 2.5 \end{pmatrix}
\]

if \( x \leq 0 \) and

\[
\begin{pmatrix}
\rho \\
m \\
E
\end{pmatrix}
= \begin{pmatrix} 0.125 \\ 0 \\ 0.25 \end{pmatrix}
\]

if \( x > 0 \). We use the Reynold’s number to be 1000 in this test. The mesh size is set to be 1000 cells and final time to be \( T = 2 \). See Figure 3.1 for the output of our simulation. We captured the rarefaction wave, contact discontinuity, and the shock well, even though the figure is smeared which is typical for a first order method.

**Example 3** (Riemann Problem) We study a Riemann problem with the following initial
conditions,
\[
\begin{pmatrix}
\rho \\
m \\
E
\end{pmatrix} = \begin{pmatrix}
0.445 \\
0.3106 \\
8.9284
\end{pmatrix}
\]
if \(x \leq 0\) and
\[
\begin{pmatrix}
\rho \\
m \\
E
\end{pmatrix} = \begin{pmatrix}
0.5 \\
0 \\
1.4275
\end{pmatrix}
\]
if \(x > 0\). The output of the numerical simulation is shown in Figure 3.2. Here, the Reynold’s number used is \(Re = 100\) with final time \(T = 2\) and on a mesh of 1000 cells.

**Example 4** (Double Rarefaction Wave) We consider an extreme Riemann problem with the following initial conditions,
\[
\begin{pmatrix}
\rho \\
m \\
E
\end{pmatrix} = \begin{pmatrix}
7 \\
-7 \\
4
\end{pmatrix}
\]
if \(x \leq 0\) and
\[
\begin{pmatrix}
\rho \\
m \\
E
\end{pmatrix} = \begin{pmatrix}
7 \\
7 \\
4
\end{pmatrix}
\]
if \(x > 0\). The exact solution contains close to a vacuum in the center. See Figure 3.3 for the numerical output with first order finite volume method. The Reynold’s number used is \(Re = 1000\) on a mesh of 1000 cells and final time \(T = 0.6\). We see low pressure and low density are both captured well as well as two rarefaction waves.
Figure 3.1  Example 2 (Lax shock tube problem). FV using 1000 uniform cells for compressible Navier-Stokes equations
Figure 3.2 Example 3 (Riemann Problem). FV using 1000 uniform cells for compressible Navier-Stokes equations
Figure 3.3 Example 4 (Double Rarefaction). FV using 1000 uniform cells for compressible Navier-Stokes equations
CHAPTER 4. SECOND ORDER FINITE VOLUME SCHEME FOR COMPRESSIBLE NAVIER-STOKES EQUATIONS

In this chapter we define the second order finite volume scheme using the reconstruction polynomials derived in Chapter 2. We then use the new second order scheme to show that density and pressure remain in the admissible set $G$ for all time levels.

4.1 Second Order Finite Volume Scheme

Recall from the first order scheme that the numerical flux is given as,

$$
\hat{F}(u_{j+1/2}^-, u_{j+1/2}^+) = \frac{1}{2}(F(u^-) + F(u^+) - \alpha(u^+ - u^-)).
$$

Note that we focus on the study for the cell interface $x_{j+1/2}$. We can then use our new definitions of $u^+$ and $u^-$ to produce a second order scheme. Thus we have

$$
\hat{f}(w_{j+1/2}^-, w_{j+1/2}^+) = \frac{1}{2} \left( f(w_{j+1/2}^-) + f(w_{j+1/2}^+) - \alpha \left( \frac{1}{2} (\rho_{j+1} + \rho_{j+2}) - \frac{1}{2} (3\rho_j - \rho_{j-1}) \right) \right)
$$

$$
\hat{g}(w_{j+1/2}^-, w_{j+1/2}^+) = \frac{1}{2} \left( g(w_{j+1/2}^-) + g(w_{j+1/2}^+) - \alpha \left( \frac{1}{2} (m_{j+1} + m_{j+2}) - \frac{1}{2} (3m_j - m_{j-1}) \right) \right)
$$

$$
\hat{h}(w_{j+1/2}^-, w_{j+1/2}^+) = \frac{1}{2} \left( h(w_{j+1/2}^-) + h(w_{j+1/2}^+) - \alpha \left( \frac{1}{2} (E_{j+1} + E_{j+2}) - \frac{1}{2} (3E_j - E_{j-1}) \right) \right)
$$
where

\[ f(w^-_{j+1/2}) = m_j + \frac{1}{2} (m_j - m_{j-1}) , \]
\[ f(w^+_{j+1/2}) = m_{j+1} + \frac{1}{2} (m_{j+1} - m_{j+2}) , \]
\[ g(w^-_{j+1/2}) = \left( \frac{1}{2} (3m_j - m_{j-1}) \right)^2 + (\gamma - 1) \left( \frac{1}{2} (3E_j - E_{j-1}) - \frac{1}{2} (3m_j - m_{j-1}) \right) , \]
\[ g(w^+_{j+1/2}) = \left( \frac{1}{2} (m_{j+1} + m_{j+2}) \right)^2 + (\gamma - 1) \left( \frac{1}{2} (E_{j+1} + E_{j+2}) - \frac{1}{2} (m_{j+1} + m_{j+2}) \right) , \]
\[ h(w^-_{j+1/2}) = \frac{3m_j - m_{j-1}}{3\rho_j - \rho_{j-1}} \left( \frac{1}{2} (3E_j - E_{j-1}) + (\gamma - 1) \left( \frac{1}{2} (3E_j - E_{j-1}) - \frac{1}{2} (3m_j - m_{j-1}) \right) \right) , \]
\[ h(w^+_{j+1/2}) = \frac{m_{j+1} + m_{j+2}}{\rho_{j+1} + \rho_{j+2}} \left( \frac{1}{2} (E_{j+1} + E_{j+2}) + (\gamma - 1) \left( \frac{1}{2} (E_{j+1} + E_{j+2}) - \frac{1}{2} (m_{j+1} + m_{j+2}) \right) \right) . \]

Thus, we can rewrite our scheme as,

\[ \rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{\Delta x} \left[ \hat{f}(w^-_{j+1/2},w^+_{j+1/2}) - \hat{f}(w^-_{j-1/2},w^+_{j-1/2}) \right] + \frac{\Delta t}{\Delta x^2} \frac{\eta}{Re} \left[ D_1(w^n_{j+1}) - 2D_1(w^n_{j}) + D_1(w^n_{j-1}) \right] , \]
\[ m_j^{n+1} = m_j^n - \frac{\Delta t}{\Delta x} \left[ \hat{g}(w^-_{j+1/2},w^+_{j+1/2}) - \hat{g}(w^-_{j-1/2},w^+_{j-1/2}) \right] + \frac{\Delta t}{\Delta x^2} \frac{\eta}{Re} \left[ D_2(w^n_{j+1}) - 2D_2(w^n_{j}) + D_2(w^n_{j-1}) \right] , \]
\[ E_j^{n+1} = E_j^n - \frac{\Delta t}{\Delta x} \left[ \hat{h}(w^-_{j+1/2},w^+_{j+1/2}) - \hat{h}(w^-_{j-1/2},w^+_{j-1/2}) \right] + \frac{\Delta t}{\Delta x^2} \frac{\eta}{Re} \left[ D_3(w^n_{j+1}) - 2D_3(w^n_{j}) + D_3(w^n_{j-1}) \right] . \]

using the above definitions for \( \hat{f}, \hat{g}, \) and \( \hat{h} \) and our previous definitions for

\[ D_1(w) = 0 , \]
\[ D_2(w) = \frac{m}{\rho} , \]
\[ D_3(w) = \frac{1}{2} \frac{m^2}{\rho^2} + \frac{3C^2}{4(\gamma - 1)P_r} . \]

The final scheme is given as,

\[ w_j^{n+1} = w_j^n - \frac{\Delta t}{\Delta x} \left[ \hat{F}(w^-_{j+1/2},w^+_{j+1/2}) - \hat{F}(w^-_{j-1/2},w^+_{j-1/2}) \right] + \frac{\Delta t}{\Delta x^2} \frac{\eta}{Re} \left[ D(w^n_{j+1}) - 2D(w^n_{j}) + D(w^n_{j-1}) \right] . \]

(4.1)

### 4.2 Positivity Limiter for the Density and Pressure

The goal is to prove that density and pressure remain in the admissible set \( G \) for all time levels using the second order finite volume scheme. It is important to note here that we can skip the diffusion term as it is already second order. We also need second order method in time
such as a high order Runge-Kutta scheme. We continue with the discussion on the inviscid terms.

Assume that \( w_{j+1/2}^-, w_{j+1/2}^+, w_{j-1/2}^-, w_{j-1/2}^+ \in G \). Observe that the first order finite volume scheme,

\[
\dot{w}_j^{n+1} = \dot{w}_j^n - \frac{\Delta t}{\Delta x} (\dot{F}(w_j^n, w_{j+1}^n) - \dot{F}(w_{j-1}^n, w_j^n))
\]

has the common argument \( w_j^n \) in each term. Our goal in this section is to rewrite the second order finite volume scheme in a similar way. Recall the second order finite volume scheme,

\[
\dot{w}_j^{n+1} = \dot{w}_j^n - \frac{\Delta t}{\Delta x} [\dot{F}(w_{j+1/2}^-, w_{j+1/2}^+) - \dot{F}(w_{j-1/2}^-, w_{j-1/2}^+)].
\]

To rewrite it in the same form as the first order scheme, we add and subtract the term \( \dot{F}(w_{j-1/2}^-, w_{j+1/2}^-) \) to obtain,

\[
\dot{w}_j^{n+1} = \dot{w}_j^n - \frac{\Delta t}{\Delta x} [\dot{F}(w_{j+1/2}^-, w_{j+1/2}^+) - \dot{F}(w_{j-1/2}^-, w_{j+1/2}^-) + \dot{F}(w_{j-1/2}^+, w_{j+1/2}^-) - \dot{F}(w_{j-1/2}^-, w_{j-1/2}^+)]
\]

\[
= \dot{w}_j^n - \frac{\Delta t}{\Delta x} [\dot{F}(w_{j+1/2}^-, w_{j+1/2}^+) - \dot{F}(w_{j-1/2}^-, w_{j+1/2}^-) - \dot{F}(w_{j+1/2}^+, w_{j+1/2}^-) + \dot{F}(w_{j-1/2}^-, w_{j+1/2}^-) - \dot{F}(w_{j-1/2}^-, w_{j-1/2}^+)].
\]

Recall that

\[
\dot{w}_j^n = \frac{1}{\Delta x_j} \int_{I_j} P_1^-(x) dx,
\]

from the derivation of the second order finite volume method. We can then write this as

\[
\dot{w}_j^n = \frac{1}{\Delta x_j} \int_{I_j} P_1^-(x) dx
\]

\[
= a_1 P_1^-(x_{j+1/2}) + a_2 P_1^-(x_{j-1/2}),
\]

where \( a_1 \) and \( a_2 \) are positive constants and \( P_1^-(x_{j+1/2}) = w_{j+1/2}^- \) and \( P_1^-(x_{j-1/2}) = w_{j-1/2}^+ \).

We can rewrite our scheme as,

\[
\dot{w}_j^{n+1} = a_1 \left( w_{j+1/2}^- - \frac{\Delta t}{a_1 \Delta x} [\dot{F}(w_{j+1/2}^-, w_{j+1/2}^+) - \dot{F}(w_{j-1/2}^+, w_{j+1/2}^-)] \right)
\]

\[
+ a_2 \left( w_{j-1/2}^+ - \frac{\Delta t}{a_2 \Delta x} [\dot{F}(w_{j-1/2}^+, w_{j+1/2}^-) - \dot{F}(w_{j-1/2}^-, w_{j+1/2}^-)] \right).
\]

Given the rewritten scheme that is in the form of the first order method, we can follow the argument exactly from the first order method to show that density and pressure remain positive for all time levels. Refer to Chapter 3 sections 3.2 and 3.3 for the discussion.

For high order methods, to ensure positivity of the pressure and density approximations, we impose a limiter. We refer to [9] on the derivation of this limiter for finite volume methods.
CHAPTER 5. CONCLUSION

In this thesis, we studied the first and second order positivity preserving finite volume methods to show that the density and pressure remain positive for all time levels \( t_n \). Given the one dimensional Navier-Stokes equations,

\[
\begin{pmatrix}
\rho \\
\rho u \\
E
\end{pmatrix}_t + \begin{pmatrix}
\rho u \\
\rho u^2 + p \\
(E + p)u
\end{pmatrix}_x = \frac{\eta}{Re} \begin{pmatrix}
0 \\
\frac{u^2}{2} + \frac{3C_a^2}{4(\gamma - 1)Pr} \\
\eta
\end{pmatrix}_x,
\]

with conservative variables \( \rho, u, \) and \( E \) as density, velocity and energy respectively, we were able to derive a first order finite volume scheme to approximate the exact solution. The first order finite volume method is given as

\[
\begin{align*}
\rho^n_j &= \rho^n_j - \frac{\Delta t}{\Delta x} \left[ \hat{f}(w^n_j, w^n_{j+1}) - \hat{f}(w^n_{j-1}, w^n_j) \right] + \frac{\Delta t}{\Delta x} \left[ D_1(w^n_{j+1}) - 2D_1(w^n_j) + D_1(w^n_{j-1}) \right] \\
m^n_{j+1} &= m^n_j - \frac{\Delta t}{\Delta x} \left[ \hat{g}(w^n_j, w^n_{j+1}) - \hat{g}(w^n_{j-1}, w^n_j) \right] + \frac{\Delta t}{\Delta x} \left[ D_2(w^n_{j+1}) - 2D_2(w^n_j) + D_2(w^n_{j-1}) \right] \\
E^n_{j+1} &= E^n_j - \frac{\Delta t}{\Delta x} \left[ \hat{h}(w^n_j, w^n_{j+1}) - \hat{h}(w^n_{j-1}, w^n_j) \right] + \frac{\Delta t}{\Delta x} \left[ D_3(w^n_{j+1}) - 2D_3(w^n_j) + D_3(w^n_{j-1}) \right]
\end{align*}
\]

where

\[
\begin{align*}
\hat{f}(w^n_j, w^n_{j+1}) &= \frac{1}{2} \left( m^n_j + m^n_{j+1} - \alpha(m^n_{j+1} - m^n_j) \right) \\
\hat{g}(w^n_j, w^n_{j+1}) &= \frac{1}{2} \left( \frac{(m^n_j)^2}{\rho^n_j} + (\gamma - 1)(E^n_j - \frac{1}{2}(m^n_j)^2) + \frac{(m^n_{j+1})^2}{\rho^n_{j+1}} \right) \\
&\quad + (\gamma - 1)(E^n_{j+1} - \frac{1}{2}(m^n_{j+1})^2) - \alpha(m^n_{j+1} - m^n_j) \\
\hat{h}(w^n_j, w^n_{j+1}) &= \frac{1}{2} \left( \frac{m^n_j}{\rho^n_j} (E^n_j + (\gamma - 1)(E^n_j - \frac{1}{2}(m^n_j)^2)) + \frac{m^n_{j+1}}{\rho^n_{j+1}} (E^n_{j+1} \right) \\
&\quad + (\gamma - 1)(E^n_{j+1} - \frac{1}{2}(m^n_{j+1})^2)) - \alpha(E^n_{j+1} - E^n_j),
\end{align*}
\]

and \( D(w) \) as defined in (3.4). We were then able to prove that density and pressure remain positive for all time levels \( t_n \). We tested the positivity preserving first order finite volume
scheme for the compressible Navier-Stokes equations using various initial conditions. We were able to show that the numerical solutions do remain positive for all time levels. We plan to fix the accuracy table so that we obtain a first order method.

We derived the second order finite volume scheme for the compressible Navier-Stokes equations using a new definition for $u^+$ and $u^-$. We obtained these new definitions by finding interpolating polynomials $P^{-1}(x)$ and $P^{+1}(x)$ such that $P^{-1}(x_{j+1/2}) \approx u^-_{j+1/2}$ and $P^{+1}(x_{j+1/2}) \approx u^+_{j+1/2}$. We then proved that density and pressure remain positive for all time levels using the second order finite volume method.

In the future, we plan to replicate the previous numerical examples to show that the second order finite volume method remains positive.

We may also consider the two dimensional compressible Navier-Stokes equations and apply first and second order finite volume methods to show that positivity is preserved for density and pressure in two dimensions. Once these are complete, we will consider the third order discontinuous Galerkin method to show density and pressure remain positive for both one and two dimensional cases.
BIBLIOGRAPHY


APPENDIX. MATLAB CODE

The MATLAB code for the first order finite volume scheme example 1 is shown below. The code for the rest of the examples is similar with different initial conditions, so it was not included.

Example 1

Nx = 500;
xmin = -5;
xmax = 5;
Re = 1000;
dx = (xmax-xmin)/Nx;
gamma = 1.4;
for i = 1:Nx
    x(i) = xmin + (i-1)*dx;
end
t = 0;
T = 2;
Pr = 0.7;
% Initial Conditions
rho_l = 1;
m_l = 0;
E_l = 2.5;
rho_r = 0.125;
m_r = 0;
E_r = 0.25;
rho(1:(Nx/2)) = rho_l;
m(1:(Nx/2)) = m_l;
E(1:(Nx/2)) = E_l;
rho((Nx/2)+1:Nx) = rho_r;
m((Nx/2)+1:Nx) = m_r;
E((Nx/2)+1:Nx) = E_r;
while t < T
    for i = 1:Nx
        p(i) = ((gamma-1)*(E(i)-(1/2)*(m(i)^2/rho(i))));
        C(i) = sqrt((gamma*p(i)/rho(i)));
        alph1(i) = abs((m(i)/rho(i))+sqrt((gamma*p(i)/rho(i))));
    end
    alph = max(alph1);
    dt = min((1/4*Nx*(Nx-1))*(1/alph)*dx, 0.001*Re*dx^2);
    if T - t < dt
        dt = T - t;
    end
    for i = 2:Nx-1
        fhr(i) = (1/2)*(m(i)+m(i+1)-alph*(rho(i+1)-rho(i)));
        fhl(i) = (1/2)*(m(i-1)+m(i)-alph*(rho(i)-rho(i-1)));
        ghr(i) = (1/2)*((m(i)^2)/(2*rho(i))*(3-gamma)+E(i)*(gamma-1)+m(i+1).^2/(2*rho(i+1))*(3-gamma)+E(i+1)*(gamma-1)-alph*(m(i+1)-m(i)));
        ghl(i) = (1/2)*((m(i-1)^2)/(2*rho(i-1))*(3-gamma)+E(i-1)*(gamma-1)+m(i).^2/(2*rho(i))*(3-gamma)+E(i)*(gamma-1)-alph*(m(i)-m(i-1)));
        hhr(i) = (1/2)*(m(i)/rho(i)*(E(i)+p(i))+(m(i+1)/rho(i+1))*(E(i+1)+p(i+1))-alph*(E(i+1)-E(i)));
        hhl(i) = (1/2)*(m(i-1)/rho(i-1)*(E(i-1)+p(i-1))+(m(i)/rho(i))*(E(i)+p(i))-alph*(E(i)-E(i-1)));
        D3(i) = (m(i+1)^2/rho(i+1)^2)*(1/2) + (3*C(i)^2/(4*(gamma-1)*Pr))
- 2*(m(i)^2/rho(i)^2)*(1/2) - 2*(3*C(i)^2/(4*(gamma-1)*Pr))
+ (m(i-1)^2/rho(i-1)^2)*(1/2) + (3*C(i)^2/(4*(gamma-1)*Pr));

rho_new(i) = rho(i) - (dt/dx)*(fhr(i) - fhl(i));
m_new(i) = m(i) - (dt/dx)*(ghr(i) - ghl(i)) + (dt/(dx^2))*((1/Re)
* ((m(i+1)/rho(i+1)) - 2*(m(i)/rho(i)) + (m(i-1)/rho(i-1))));
E_new(i) = E(i) - (dt/dx)*(hhr(i) - hhl(i)) + (dt/(dx^2))*((1/Re)*(D3(i)));

end

rho_new(1) = rho(1);
m_new(1) = m(1);
E_new(1) = E(1);
rho_new(Nx) = rho(Nx);
m_new(Nx) = m(Nx);
E_new(Nx) = E(Nx);
rho = rho_new;
m = m_new;
E = E_new;
t = t + dt;
end

u = m_new./rho_new;

subplot(3,1,1)
plot(x,rho_new,’-’)
xlabel(’x’)
ylabel(’Density’)
figtitle = (’Density’);
title(figtitle)
legend(’Numerical solution’,’Exact solution’,’Location’,’Best’)

subplot(3,1,2)
plot(x,u,’-’)
xlabel(’x’)
ylabel('Velocity')

figtitle = ('Velocity');
title(figtitle)

legend('Numerical solution','Exact solution','Location','Best')

subplot(3,1,3)

plot(x,p,'-')

xlabel('x')

ylabel('Pressure')

figtitle = ('Pressure');
title(figtitle)

legend('Numerical solution','Exact solution','Location','Best')

set(gcf,'Color','white')