Supersonic Flow Simulation with Entropy-Based Artificial Viscosity Stabilization

BY

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THESIS

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To my parents,
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The completion of this research work would not have been, without a doubt, possible without the professional guidance and personal comradery of others.

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HA
Contribution of Authors

Chapter 1 and 2 present a literature review that places my dissertation question in the context of the larger field and highlights the significance of my research question. Chapter 3 and 4 mainly are mainly focused on the mathematical formulation and the discretization of the governing equations which bears a close resemblance to the original work of Gustaaf Jacobs [1, 2]. Chapter 5 entails the details of my developed model for supersonic flow simulation in gas dynamics. The results of this section of the work which I was the primary contributor is published in the journal of Computers and Fluids [3]. I was the primary author of the manuscript, however, Professor Farzad Mashayek and Professor Gustaaf Jacobs, my Ph.D. research advisors, reviewed the manuscript and made constructive comments. Chapter 6 is focused on the extension of the model to viscous and turbulent flow simulation and contains unpublished results. The findings of this part of research are written in another manuscript, written mainly by myself, and is expected to appear in Physics Letters A. Again, Professor Farzad Mashayek and Professor Gustaaf Jacobs assisted me in writing the manuscript through several rounds of review and making comments on the paper structure and content.
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SUMMARY

High-fidelity simulation of supersonic flows is a powerful tool for gaining insight into the complex physics of such flows at a fraction of cost and time of experiments. The availability of supercomputers has made massively parallel numerical simulations a viable option and has inspired a vast amount of research efforts to develop accurate and affordable numerical tools for simulation of real world engineering problems.

The accurate simulation of supersonic flows is well suited to higher-order computational fluid dynamics (CFD). Since these cases often involve flow accompanied by strong shock waves, an appropriate shock capturing technique for higher-order methods is necessary. Among the numerous available methods for shock capturing, adding artificial viscosity seems to be the most promising option which has been successfully implemented in classical numerical schemes, e.g. finite volume methods. In this research we embark upon the implementation of an artificial viscosity shock capturing technique in a high-order discontinuous Galerkin (DG) method to accurately simulate shock dominated flows.

The artificial viscosity model used in this work is a modified form of the entropy viscosity (EV) method. The artificially added viscosity is proportional to the local size of an entropy production. The entropy satisfies a conservation equation only in the regions where the solution is smooth and satisfies an inequality in shocks. The basic idea used in entropy viscosity method is based on the assumption of a large entropy production at shocks. Since the residual of an entropy equation is supposed to be vanishingly small in smooth regions and large in shocks, the
dissipation will be virtually added only to shocked regions. However, direct implementation of the entropy viscosity method in our discontinuous spectral element method (DSEM) leads to a non-smooth artificial viscosity, which in turn leads to oscillations and instability of the solution. To smooth the artificial viscosity, the EV method is coupled with a spectral filter and an interface treatment technique. The resulting artificial viscosity is locally large near discontinuities and transitions smoothly to zero in smooth flow regions. The method enables using elements with orders higher than unity while avoiding adaptive mesh refinement and preserving the locality and compactness of the DG scheme.

Since supersonic flows are, by definition, high speed and naturally turbulent, the shock capturing method should be capable of resolving shocks in presence of turbulence. Consequently, the use of the method is extended to compressible turbulence and a special emphasis is placed on distinguishing strong oscillations associated with turbulence from shock waves. A modified formulation incorporating a shock sensor is proposed for turbulent flows and the obtained results confirm the ability of the modified method to capture shocks while preserving the main features of the turbulence structure.
CHAPTER 1

INTRODUCTION

1.1 Motivation

Future high-speed aircrafts for long-range passenger transportation and current demand for space and military applications requires the development of efficient supersonic propulsion systems. A supersonic combustion ramjet, i.e. scramjet, is one of the most prominent technologies for realizing supersonic flight and transportation capabilities. Recent successful flights of X-43A [6] and X-51A [7], have proven the potential and made the scramjet one of the most promising air breathing supersonic propulsion technologies and have drawn an ever increasing attention of researchers worldwide [8,9]. It is needless to say, scramjet engines still have many unresolved fundamental issue to overcome. Some of the main difficulties can be traced to the lack of a detailed physical understanding and accurate prediction of supersonic combustion.

In general, the scramjet engine consists of an inlet, an isolator, a combustor and a nozzle. The combustor is the main component for the design of a scramjet engine, since the mixing and ignition processes occur mainly in this section. Compared to an ordinary jet engine operating at subsonic speeds, the design of supersonic combustor is more challenging and involves several complexities. First, the residence time of the fuel in the supersonic combustor is very short, of the order of millisecond [10]. In addition to short residence time of air and fuel in the combustor, concurrent presence of shock waves, turbulence and chemical reaction gives rise to
a very complex multi-scale and multi-physics problem. Therefore, a detailed study and thorough knowledge of supersonic turbulent fluid flow; reaction mechanisms and their interactive effects are of crucial importance for the ultimate success of a scramjet engine design.

To gain such understanding, two approaches can be envisioned, experimental studies and numerical simulation. Although, experimental studies are still an inevitable element of the design process, with the recent advances in computer technologies and numerical techniques, computer simulations have become a viable alternative to experiments, providing insight into the physics of such problems at a fraction of cost and time.

The main motivation behind this work is the interest in analyzing supersonic turbulent flow in scramjet engines using high-fidelity numerical simulations. The specific goal of this research is the development of a novel numerical method for high-fidelity simulation of supersonic and turbulent fluid flow. The method sought for is ideally capable of locating strong shocks and capturing them within the numerical stencil and also resolving wide range of turbulence time and length scales. Special consideration is given to efficient and accurate modeling of shock and turbulence interaction, a significant challenge in supersonic turbulence simulation.

1.2 Simulation of Supersonic Turbulent Flows

Flow in a scramjet is just an example from the wide spectrum of industrial and scientific applications where the flow is both supersonic and turbulent. Some other applications include; inertial confinement fusion, supernovae explosion and lithotripsy [11][12]. Shock waves and other flow discontinuities along with turbulence are present concurrently in supersonic turbulent flows and interact with each other dynamically. Shocks waves are extremely thin regions of widths on
the order of a few mean free paths; where the flow experiences sudden change in its properties.

Turbulence, on the other hand, is an unpredicted and somewhat random process with wide
ranges of time and length scales. As a result, analytical solutions do not exist to this problem.
However, numerical simulations can provide acceptable prediction of turbulence behavior in
many cases. A numerical solution to Navier-Stokes system of equations in which all the dynamic
length scales of the flow are resolved is called direct numerical solution (DNS). Though it is
accurate, DNS requires excessive computational cost to resolve the all turbulence scales, which
makes its range of application limited.

A significant challenge in simulation of supersonic turbulent flows is to establish a numerical
scheme that is able to accurately simulate flows involving flow discontinuities, turbulence and
their interactions. The difficulty arises from the contradictory properties of numerical methods
designed to treat shocks and turbulence where the numerical scheme needs to satisfy two com-
peting requirements: capturing different types of discontinuities and simultaneously resolving
the broadband scales of turbulence.

In order to represent the flow discontinuities in an accurate fashion over a numerical grid,
the numerical scheme needs to smear the discontinuity to some extent in order to capture it over
a few grid points by adding artificial dissipation. These methods are called shock capturing.
However, the use of a shock-capturing scheme can crucially affect the fidelity of the solution. A
poorly designed shock capturing method can be too dissipative and smear the solutions, overly
dissipate turbulence, and thus lead to an inaccurate representation of the flow discontinuities
and turbulence. The objective of the present research is to design an accurate shock capturing
method using high-order numerical methods.

1.3 Shock Capturing in High-order Numerical Methods

1.3.1 High-order Numerical Methods

A finite volume method (FVM) is the industry standard approach to computational fluid
dynamics (CFD) for compressible shock-dominated flows [13]. Despite the significant growth in
computational resources, high-order methods are still not favored in the FVM community and
second-order accurate methods are most prevalent. High-order methods are typically more ac-
curate and provide more flexibility in terms of application to real-world problems with complex
geometries and shapes. In this work we use a staggered grid discontinuous spectral element
method (DSEM) which is a discontinuous Galerkin (DG) method. The DG method was first
introduced in 1970s by Reed and Hill [14] for neutron transport equation and was first used
by Cockburn and Shu [15] in the field of CFD for Euler equations solution in the early 1990s.
Bassi and Rebay [16] were the first researchers to apply the DG formulation to the Navier-Stokes
systems of equations reporting promising results. During the past two decades, discontinuous
Galerkin (DG) methods have increasingly become a viable alternative in the field of computa-
tional fluid dynamics and have been adapted to study compressible and incompressible, steady
and unsteady, as well as laminar and turbulent flows [17–19].

The DG method combines the properties of high-order discretization of the Galerkin finite
element method and the local conservation typical of the finite volume methods. Furthermore,
the discretization offers advantages in terms of local mesh adaptation and efficient paralleliza-
tion \textsuperscript{20,28}. DSEM approximates the solution variables of conservation laws through a high-order local basis function in non-overlapping elements that may be oriented arbitrarily within an unstructured grid. Within each element, the solution is approximated by a polynomial of degree $P > 0$, while the continuity conditions at the element interfaces are relaxed (as in FVM). The local, non-overlapping nature of the elements not only enables meshing of flow geometries of any complexity; it also ensures a high parallel efficiency and easy boundary condition implementation. DSEM has very small diffusion and dispersion errors and is spectrally convergent if the solution is smooth \textsuperscript{20,21}. In addition to being arbitrarily high order accurate, the DG method also permits the formulation of very compact numerical schemes. This characteristic makes this method extremely flexible in the sense of easily handling a wide variety of element types, and also allows a number of adaptive techniques like h– or p–refinement or both \textsuperscript{20,30}.

1.3.2 Shock Capturing

As discussed earlier, shock waves are very thin layers of drastic changes in the properties of the flow. The thickness of such a layer is of the order of the mean free path of the molecules, which is approximately $10^{-5}$ cm. As a result, the behavior of the flow within the interior of shock waves is of no significant importance from a macroscopic point of view. Therefore, shock waves are mathematically treated as discontinuities and represented with a jump of all fields of flow. This representation of the flow discontinuities can cause trouble in high-order numerical methods. In specific, the implementation of DG methods for flows with discontinuities, such as supersonic flows, has proven quite challenging. Specifically, higher order approximations of discontinuous shock solutions that appear if the flow is supersonic, are troubled by spurious
unphysical oscillations in the region of flow discontinuities, known as Gibbs oscillations \cite{23}. Numerical schemes designed to solve the system of governing equations must be able to capture any discontinuity that might arise in the solution. There has been an abundance of work on extension of classical shock capturing methodologies to high-order methods. They can be broadly categorized as the use of limiters \cite{31}, the weighting of stencils such as essentially non-oscillatory (ENO) and weighted essentially non-oscillatory (WENO) schemes \cite{32, 33} and the addition of artificial viscosity in the vicinity of shocks. Each of these methods is based on the smoothing of the solution local to the shock with the objective to essentially or entirely removing Gibbs oscillations.

Despite their indisputable success, the use of limiters in high-order DSEM approximations is challenging. Moreover, the use of limiters tends to drastically reduce the accuracy in a wide region near the shock. Similarly, the extension of non-oscillatory numerical algorithms to complex geometries is complicated \cite{34-36}. These methods reconstruct high-order approximations of the solution away from the discontinuities while resolving sharp profiles using additional degrees of freedom (DOF). However, they usually require carefully chosen reconstruction and numerical fluxes and their computational overhead for high-order approximations is high. Extension to multiple dimensions is limited to structured meshes.

1.3.3 Artificial Dissipation

Another approach to stabilize high-order numerical schemes is by adding diffusion to remove non-physical oscillations near shocks. Although this enables the capturing of the shocks and discontinuities, the diffusion near the sharp discontinuities may easily be excessive and tends
to grow over time. Moreover, since viscosity is applied over the entire domain, one may lose the benefit of high order resolution. A method capable of adding viscosity which is localized in regions of shock, limited at contact discontinuities and virtually zero in smooth regions is desirable.

Von Neumann and Richtmeyer [37] introduced the idea of a nonlinear artificial viscosity. This concept was adopted later by Baldwin and MacCormack [38] to simulate the interaction of shock waves with turbulent boundary layer. Later Jameson et al. [39] used this approach in the context of finite volume in combination with a Runge-Kutta time stepping scheme to simulate compressible flows in complex geometries. Adding artificial viscosity has long been the preferred method of shock capturing in the context of streamwise upwind Petrov-Galerkin (SUPG) finite element methods, as proposed by Hughes et al. [40]. Researchers such as Hartmann and Houston [41] and Aliabadi et al. [42] have used artificial viscosity for shock capturing with DG, albeit only for polynomial order $P = 1$ solutions. Although this method, and other similar methods, are capable of adding the required amount of viscosity near shocks to spread the discontinuity and also control the numerical oscillations behind the shock wave, they can in turn overly diffuse the waves and produce incorrect wave speeds.

There have been other attempts to particularly design algorithms to add artificial viscosity to high-order discontinuous Galerkin methods. Persson and Peraire [43] introduced a polynomial order dependent artificial viscosity to produce sub-cell shock resolution for discontinuous Galerkin schemes. To locate the shocks in the flow field, Persson and Peraire developed a sensor based on the magnitude of the highest-order coefficients in an orthonormal representation of
the solution. Later, Barter and Darmofal [44] used a reaction-diffusion equation to obtain a viscosity that is smooth in both time and space. Reinser et al. [45] used a similar reaction-diffusion equation in combination with the gradient based classical artificial viscosity to achieve a space-time smooth viscosity. Unfortunately, to achieve sufficient smoothing of the viscosity, one needs to choose a large diffusivity coefficient, which results in a stiff system of ODEs for time integration. The resulting time step restriction can be handled through implicit time integration. Implicit time stepping, however, not only is more laborious to implement, it also is more expensive per time step, and less parallel efficient for parallel computing.

Recently, Guermond et al. [46] proposed an artificial viscosity method for spectral methods, based on the local rate of entropy generation. In this method, the magnitude of the artificial viscosity is coupled to the magnitude of entropy generation. Since shocks generate entropy, the magnitude of entropy generation not only identifies the shock, but also is an excellent measure for the magnitude of the artificial viscosity. Hence, the addition of a numerical dissipation term proportional to the local entropy production rate contributes a numerical dissipation to the shock regions and hence removing Gibbs oscillations, while virtually no dissipation is added in the regions far from the shock to ensure an accurate computation of small-scale, turbulent flow away from shocks. In [46] the EV method was shown to be stable and accurate in combination with a continuous spectral element method. Zingan et al. [47] extended the use of EV to discontinuous finite element method, which is limited to the use of relatively low-order elements.
1.4 Thesis Overview

This work explores the feasibility of the entropy viscosity method within the framework of staggered grid DSEM. The standard entropy viscosity model was not designed for implementation in conjunction with a discontinuous collocation method. Specifically, element-to-element jumps in artificial viscosity leads to oscillations in solution gradients which can corrupt the smoothness and accuracy of the downstream flow field. We develop a smooth artificial viscosity by employing an elemental level filter and an interface treatment technique that results in a space-time smooth artificial viscosity. This artificially added coefficient is large and localized near discontinuities and transitions smoothly to zero in smooth flow regions. The method works in conjunction with high-order elements, avoiding adaptive mesh refinement, and preserves the locality and compactness of the DG scheme. Moreover, we present a modified formulation of our method for turbulent flows governed by the Navier-Stokes system of equation. This methodology enables us to extend the use of EV method to turbulent viscous flows and generalizes the method’s application to situations where there are strong physical oscillations like those associated with turbulence.

The thesis is organized as follows: A brief background on hyperbolic conservation laws is given in Chapter 2, where we will also review the main idea of stabilization of numerical solutions using artificial dissipation. Chapter 3 reviews the system of compressible Navier-Stokes equations and presents a brief discussion on entropy transport in gas dynamics and viscous fluid flow systems. In Chapter 4, we present the details of our numerical methodology. Chapter 5 is dedicated to discussion on the implementation of entropy viscosity method in
DSEM. In the same chapter we explain the general algorithm of the numerical scheme for shock capturing. Chapter 5 also explores the performance of DSEM-EV in dynamically capturing the discontinuous solution in one-dimensional and two-dimensional compressible flows governed by Euler equations. We discuss the extension of the method to Navier-Stokes system of equations in general, and to turbulent flows in particular, in chapter 6. The final chapter is reserved for conclusions and recommendations for future work.
CHAPTER 2

DISCONTINUOUS FLOWS AND THE IDEA OF NUMERICAL STABILIZATION WITH ARTIFICIAL VISCOSITY

The purpose of this chapter is to provide a succinct presentation of mathematical properties of conservation laws responsible for shock wave formation. In this chapter, we restrict our attention to simple model problems. We look into the mathematical difficulties encountered in shocked systems and present a remedy based on the entropy properties which forms the building block of our shock capturing methodology.

2.1 Conservation Laws with Discontinuous Solution: Basic Concept

2.1.1 Shock Formation

Here we study some distinguished features of conservation laws, such as wave steepening and shock formation [4]. The nonlinear hyperbolic conservation laws are known to produce discontinuities in the solution, even if the initial data is smooth. In order to mathematically illustrate this mechanism we consider a one-dimensional initial value problem (IVP) for scalar non-linear conservation law, namely

\[ \partial_t u + \partial_x f(u) = 0, \quad u(x,0) = u_0(x) \]
The flux function $f$ is assumed to be a differentiable function of the solution $u$ which allows us to re-write the IVP equation in the following form:

$$\partial_t u + \lambda(u) \partial_x u = 0 \quad (2.2)$$

where

$$\lambda(u) = \frac{df}{du} = f'(u) \quad (2.3)$$

is called the *characteristic speed* which is the eigenvalue of the Jacobian matrix. For the linear advection equation, $\lambda(u) = a$ and the solution is simply $u(x,t) = u_0(x - at)$ for $t \geq 0$. As time evolves, the initial data simply propagates unchanged with velocity $a$. The solution $u(x,t)$ is then constant along each ray $(x - at) = x_0$, which are known as the *characteristic* of the equation. In general, if we seek a curve $x = x(t)$ in the $x-t$ plane such that $u(x(t), t) = \text{const}$, we can write

$$\frac{du(x(t), t)}{dt} = \frac{\partial u(x(t), t)}{\partial t} + \frac{\partial u(x(t), t)}{\partial x(t)} \frac{dx(t)}{dt} = 0 \quad (2.4)$$

which implies

$$\frac{dx(t)}{dt} = f'(u(x(t), t)) \quad (2.5)$$

Taking into account the fact that $u$ is constant along each curve we can say $u(x(t), t) = u(x(0), 0) = u_0(\chi) = \text{const}$ where $x(0) = \chi$. [Equation 2.5] can be written as an ODE

$$\frac{dx(t)}{dt} = f'(u_0(\chi)), \quad x(0) = \chi \quad (2.6)$$
A solution of the form $x = \chi + f'(u_0(\chi)) t$ satisfies the ODE presented above and represents a characteristic of the PDE under discussion. In general, $f'(u_0(\chi))$ is the characteristic speed which as mentioned before is a constant value for the linear advection equation. In this particular case, the family of characteristics all have the same slope and never cross each other. However, if $f(u)$ is a nonlinear function of $u$, such as for the Burgers equation, for which $f(u) = \frac{1}{2} u^2$, some different characteristics may cross over, originating an infinite slope in the solution $u(x,t)$ and forming a shock wave. We suppose this happens at a precise time $T_{\text{shock}}$.

For times $t < T_{\text{shock}}$, we can use Equation 2.5 and Equation 2.6 to find the classical solution of the IVP. However, for $t > T_{\text{shock}}$ some of the characteristics have crossed and so there are points $x$ where there are several characteristics leading back to $t = 0$ and therefore there may not be an unique solution for $u$ which necessitates the solution to be a multi-valued function. For most physical situations this does not make sense; for example, the density of a gas cannot possibly be multi-valued at a point.

This is an anomalous situation that may be rescued by going back to the physical origins of the equations and investigating the adequacy of the model for the physics of the problem. Relevant physical phenomena of interest here are shock waves in compressible media which have viscous dissipation and heat conduction, while, the model furnished by Equation 2.1 does not cover such effects. Adopting the vanishing viscosity approach allows us to determine the correct physical behavior and define a nonclassical or generalized solution of the equation.
2.1.2 Vanishing Viscosity Approach

One way to introduce a generalized solution of the hyperbolic scalar conservation law Equation 2.1 is to replace the flux term with a more appropriate function which also includes a dependence on $u_{xx}$ in addition to the solution

$$\partial_t u + \partial_x f(u) = \epsilon u_{xx}, \quad u(x, 0) = u_0(x) \quad (2.7)$$

Figure 1: Shock formation in inviscid Burgers equation.

where $\epsilon$ is a positive coefficient of viscosity. The modified model indicates that the time rate of change of $u$ is a competing balance between advection and diffusion terms rather than being purely governed by advection. Equation 2.1 is a model of Equation 2.7 valid only for small $\epsilon$ and
smooth $u$. If the initial data is smooth and $\epsilon$ very small, then before the solution is shock free the $\epsilon u_{xx}$ term is negligible compared to the other terms and we might expect the solution to both PDEs to be very close and look nearly identical. If a shock wave starts to form, the gradients of the solution start to rapidly increase and as a result the second derivative term $u_{xx}$ grows much faster than $u_x$ and at some point the $\epsilon u_{xx}$ becomes comparable to the other terms and plays a role in keeping the solution smooth. Figure 2 shows a comparison between the behavior of inviscid and viscous Burger’s equation as the discontinuity is replaced by a smooth continuous function as a result of adding small values of $\epsilon$. As $\epsilon \to 0$ the function becomes sharper and approaches the discontinuous solution. This is the main idea behind adding artificial viscosity to shocked and discontinuous flows where we want to keep the dissipation negligible away from the shocks and very small at discontinuities to achieve a smooth solution.

2.1.3 Weak Solutions

Another way to define a generalized solution of the inviscid Equation 2.1 is to go back to the more fundamental integral form of conservation law, which does not require the differentiability of the integrands. A more convenient approach is to take the PDE, multiply by a smooth test
function, integrate one or more times over some domain, and then use integration by parts to move derivatives off the function $u$ and onto the smooth test function, $\phi(x,t)$. The result is an integral equation involving fewer derivatives on $u$, and hence requiring less smoothness. By doing this operation and integrating over time and space:

$$\int_0^\infty \int_{-\infty}^\infty [\phi \partial_t u + \phi \partial_x f(u)] \, dx \, dt = 0 \quad (2.8)$$

now integrating by parts yields:

$$\int_0^\infty \int_{-\infty}^\infty [\phi \partial_t u + \phi \partial_x f(u)] \, dx \, dt + \int_{-\infty}^\infty \phi(x,0) u(x,0) \, dx = 0 \quad (2.9)$$

Note that nearly all the boundary terms that normally arise through integration by parts drop out. The remaining boundary term brings in the initial condition of the PDE. The above formulation is called the \textit{weak integral formulation} and we say the solution $u$ of the conservation equation is a \textit{weak solution} if it satisfies the integral form for all test functions $\phi$.

The vanishing viscosity generalized solution we defined in the previous section is a weak solution in the sense of Equation 2.9. However, we should note that weak solutions are often not unique and so an additional condition should be sought for to determine which weak solution is the physically correct vanishing viscosity solution. The condition one can impose to pick out the correct solution is called \textit{entropy conditions} and consequently the vanishing viscosity solution is also called the entropy solution. In the next subsections we demonstrate this fact.
by considering the one-dimensional Riemann problem as an example of nonuniqueness of weak solution.

2.1.4 Riemann Problem

The conservation law together with a piecewise constant data having a single discontinuity is known as the Riemann problem \[48\]. Consider a scalar conservation law \( \partial_t u + \partial_x f(u) = 0 \) with initial data

\[
    u_0(x) = \begin{cases} 
        u_L, & \text{if } x < 0 \\
        u_R, & \text{if } x > 0 
    \end{cases} \tag{2.10}
\]

where \( u_L \) and \( u_R \) are two constant values and the initial data has a discontinuity at \( x = 0 \). Obviously, there are no classical solutions to this IVP. Two different scenarios can be envisioned. If \( u_L > u_R \), then at any given time and any spatial location \( f'(u_R)t < x < f'(u_L)t \) the solution will be multi-valued. If \( u_L > u_R \), at any given time the solution is not defined for \( f'(u_L)t < x < f'(u_R)t \). To find the non-classical or generalized solution of the IVP, one should consider the relation between \( u_R \) and \( u_L \).

**Case I:** \( u_L > u_R \)

In this case we expect the initial discontinuity to propagate with a speed of \( s \) and thus represent a particular characteristic curve \( x = st \). This curve separates two different sets of characteristic curves to its right and left. The solution on curves to the left, takes on the value
$u_L$ and on those to the right takes on the value $u_R$. So the solution to the Riemann problem in this case is simply

$$u(x,t) = \begin{cases} u_L, & \text{if } x - st < 0 \\ u_R, & \text{if } x - st > 0 \end{cases} \quad (2.11)$$

which represents a right traveling shock with a speed of $s$. Note that characteristics in each of the regions where $u$ is constant go into the shock as time evolves (See ??).

In a general case, the shock speed $s$ is a time dependent variable but in the case of the Riemann problem it can be shown that $s$ is only a function of the right and left states. The speed of propagation can be determined by conservation. Consider a one-dimensional scalar equation in its integral form between two arbitrarily chosen times $t_1$ and $t_2$

$$\int_{x_1}^{x_2} u(x,t_2)dx - \int_{x_1}^{x_2} u(x,t_1)dx + \int_{t_1}^{t_2} f(u(x_2,t))dt - \int_{t_1}^{t_2} f(u(x_1,t))dt = 0 \quad (2.12)$$

where $x_1$ and $x_2$ are the shock locations at times $t_1$ and $t_2$, respectively. The above equation can be modified as follows:

$$u_L \Delta x - u_L \Delta x + f(u_R) \Delta t - f(u_L) \Delta t = 0 \quad (2.13)$$

which gives

$$s = \frac{\Delta x}{\Delta t} = \frac{f(u_L) - f(u_R)}{u_L - u_R} = \frac{[f]}{[u]} \quad (2.14)$$
the above relation is called Rankine-Hugoniot jump condition and gives the relation between
the shock speed and the states $u_L$ and $u_R$ for any arbitrary flux function $f(u)$. Although, in
the case of simple Riemann problem presented in this section, the shock speed is constant but
in a more general case, the Rankine-Hugoniot conditions hold across any propagating shock,
where now $u_L$ and $u_R$ are the values immediately to the right and left of the discontinuity and
$s$ is the corresponding instantaneous shock speed.

**Case II:** $u_R > u_L$

In this case there are infinitely many weak solutions. One of these solution is again, Equation 2.11 and Equation 2.14. However, this weak solution is not stable to perturbations - if the
initial data is smeared out slightly, or if a small amount of viscosity is added to the equation,
the weak solution changes completely. The physically relevant weak solution is the rarefaction
wave in this case as depicted in ??.

\[ u(x, t) = \begin{cases}
  u_L, & x < u_L t \\
  x/t, & u_L t \leq x \leq u_R t \\
  u_R, & x > u_R t
\end{cases} \tag{2.15} \]

### 2.1.5 Entropy Conditions

As it was mentioned earlier, there are situation in which the weak solution is not unique
and an additional condition is needed to pick out the physically relevant viscosity vanishing
solution. Often the condition which defines the solution is simply that the weak solution must
be the vanishing viscosity solution to the proper viscous equation. However, this condition is hard to work with directly and instead, other conditions have been proposed to be applied to weak solution in order to check their admissibility. The main criteria that is used here, is called **entropy conditions**. The condition has its roots in the second law of thermodynamics which states that the entropy of a system must be constant or increasing with time. This provides a perfect measure to distinguish between a physically admissible shock and a spurious or expansion shock. Across a physical shock the entropy increases suddenly, whereas, in a spurious shock the entropy decrease which is the reason for rejecting the solution. When dealing with gas dynamics, the entropy can be computed as a function of pressure and density and the behavior of entropy can be used to test a solution for admissibility. We will go over this concept in details in the next chapters. Similarly, for a one-dimensional scalar conservation law one can define an entropy function, \( \eta(u) \), which bears similar diagnostic properties. In gas dynamics, the entropy is constant along particle paths in smooth flow for which an additional conservation law holds for smooth solution that becomes an inequality for discontinuous solutions. For a scalar equation, we find that if the solution \( u \) is smooth then the entropy function \( \eta(u) \) satisfies an additional differential equation

\[
\partial_t \eta(u) + \nabla \cdot \phi(u) = 0 \tag{2.16}
\]

where \( \phi(u) \) is entropy flux. Moreover, if \( \eta \) and \( \phi \) are smooth and differentiable, we may write:

\[
\eta'(u) \partial_t (u) + \phi'(u) \nabla \cdot u = 0 \tag{2.17}
\]
the conservation law can be written as \( \partial_t \eta(u) + f'(u) \nabla \cdot u = 0 \). Multiplying this equation by \( \eta'(u) \) and comparing with Equation 2.17 we can obtain

\[
\phi'(u) = \eta'(u)f'(u)
\]

(2.18)

for a scalar conservation law this equation admits many solutions \( \eta(u) \) and \( \phi(u) \). Now, for the reasons that will be seen below, let’s assume that the entropy function is convex, i.e. \( \eta'' > 0 \) for all \( u \). The derivations presented so far does not hold true for a non-smooth flow as the entropy is not conserved in such flows. Since, we are considering the vanishing viscosity solution as a replacement for the discontinuous solution, it is justified to look at the related viscous problem and study the behavior of entropy in this context.

Since the solution to the viscous problem Equation 2.7 is always smooth, we can follow the same strategy presented above to derive the evolution equation for the entropy. Multiplying Equation 2.7 by \( \eta'(u) \) yields:

\[
\eta'(u) \partial_t u + \eta'(u) \nabla \cdot f(u) = \epsilon \eta''(u) u_{xx}
\]

(2.19)

or

\[
\partial_t \eta(u) + \nabla \cdot \phi(u) = \epsilon \nabla \cdot (\eta'(u) \nabla \cdot u) - \epsilon \eta''(u) u_x^2
\]

(2.20)
Integrating this equation over an arbitrarily chosen rectangle \([x_1, x_2] \times \,[t_1, t_2]\) gives:

\[
\int_{t_1}^{t_2} \int_{x_1}^{x_2} \left[ \partial_t \eta(u) + \nabla \cdot \phi(u) \right] \, dx \, dt = \epsilon \int_{t_1}^{t_2} \int_{x_1}^{x_2} \nabla \cdot (\eta'(u) \nabla \cdot u) \, dx \, dt - \int_{t_1}^{t_2} \int_{x_1}^{x_2} \eta''(u) u_x^2 \, dx \, dt \tag{2.21}
\]

The first term on the right hand side vanishes as \(\epsilon \to 0\). This is clearly true if \(u\) is smooth at \(x_1\) and \(x_2\). If the weak solution is discontinuous at any spatial point or any time, the first term will still vanish because the double integral is bounded. The other term, on the other hand, involves integrating \(u_x^2\) and does not vanish if the weak solution is not smooth. However, since \(\epsilon > 0\), \(u_x^2 > 0\) and \(\eta'' > 0\), we can conclude that it approached a non-negative limit, as \(\epsilon \to 0\):

\[
\int_{t_1}^{t_2} \int_{x_1}^{x_2} \left[ \partial_t \eta(u) + \nabla \cdot \phi(u) \right] \, dx \, dt \leq 0. \tag{2.22}
\]

Since the integral limits were chosen arbitrarily, we can claim the integrand should have the same property as the integral:

\[
\partial_t \eta(u) + \nabla \cdot \phi(u) \leq 0. \tag{2.23}
\]

Consequently, it is observed that the entropy function of the conservation law under discussion is not necessarily conserved, but can only decrease. Note that our mathematical assumption of convexity leads to an entropy function that decreases, whereas the physical entropy in gas dynamics can only increase. To summarize, we admit the entropy inequality as our entropy condition and say a weak solution \(u(x, t)\) of the hyperbolic conservation law is an entropy solution if the entropy condition is satisfied in the weak sense. This is a key ingredient for development
of the numerical schemes for solving conservation equations with discontinuities in which we solve the equivalent viscous equation.

2.2 Numerical Stabilization by Artificial Viscosity

In the previous section we introduced the concept of vanishing viscous solution and we observed that the discontinuous solution of conservation law can be replaced with a weak solution which itself was to solution of the generalized or perturbed conservation equation. The perturbation term appears as a dissipation term and it prevents the discontinuity from “breaking down”. In this section we demonstrate the inclusion of such a dissipation term via regularization of simple one-dimensional conservation equations. We first derive the criteria of numerical stability for a certain primitive numerical scheme. Then we introduce the basic recipe for entropy-based artificial viscosity and present some one-dimensional test cases to showcase its performance.

2.2.1 Von Neumann Stability Analysis

Let’s consider the linear advection equation in one space dimension:

\[ \partial_t u + c \partial_x u = 0, \quad u(x, 0) = u_0(x) \]  \hspace{1cm} (2.24)

to which we know the solution:

\[ u(x, t) = u_0(x - ct) \]  \hspace{1cm} (2.25)

which is the classical solution if the initial data is smooth and the entropy admissible solution
to the generalized problem in case of a non-smooth initial condition as shown in Figure 3. The perturbed or regularized counterpart of this equation is represented by

$$\partial_t u + c \partial_x u = \epsilon \partial_{xx} u$$  \hspace{1cm} (2.26)

Let us now consider this equation and investigate the effect of $\epsilon$ on the stability of a well known numerical scheme to solve this problem numerically. We choose a centered difference scheme for simplicity and discretize the regularized equation in space and time:

$$\frac{u_{h,i}^{n+1} - u_{h,i}^n}{\tau} + c \frac{u_{h,i+1}^n - u_{h,i}^n}{2h} = \epsilon \frac{u_{h,i-1}^{n+1} - 2u_{h,i}^n + u_{h,i+1}^n}{h^2}$$  \hspace{1cm} (2.27)
or
\[ u_{h,i}^{n+1} = \frac{\tau}{h} \left( \frac{c}{2} + \frac{\epsilon}{h} \right) u_{h,i-1}^n + \left( 1 - \frac{2\epsilon \tau}{h} \right) u_{h,i}^n + \frac{\tau}{h} \left( -\frac{c}{2} + \frac{\epsilon}{h} \right) u_{h,i+1}^n \] (2.28)

The above equations serves as a sample algorithm to solve the conservation equation numerically. Now, we perform a Von Neumann analysis to determine within which range of variation of \( \epsilon \) the numerical scheme is stable. The numerical solution \( u_h \) can be expanded in the orthonormal basis \( \{ e^{Imx} \}_{m=-\infty}^{+\infty} \) as follows:
\[ u_h = \sum_{m=-\infty}^{+\infty} C_m(t^n)e^{Imx} \] (2.29)
where \( C_m(t^n) \) is an \( m^{th} \) complex amplitude at time \( t^n \) and \( I = \sqrt{-1} \). By substituting Equation 2.29 in Equation 2.28 we can write:
\[ C_{m+1}^{n+1} = \left( \frac{\tau}{h} \left( \frac{c}{2} + \frac{\epsilon}{h} \right) e^{-Imh} + \left( 1 - \frac{2\epsilon \tau}{h} \right) + \frac{\tau}{h} \left( -\frac{c}{2} + \frac{\epsilon}{h} \right) e^{+Imh} \right) C_m^n \] (2.30)

using the Euler formula
\[ e^{Ix} = \cos x + I \sin x \] (2.31)

simplifies Equation 2.32 to:
\[ C_{m+1}^{n+1} = \left( 1 - \frac{2\epsilon \tau}{h^2} (1 - \cos mh) - I \frac{\epsilon \tau}{h} \sin mh \right) C_m^n \] (2.32)
for stability the term inside the parentheses has to be less or equal unity which necessitates:

$$\epsilon^2 - \frac{h^2}{\tau(1 - \cos mh)} \epsilon + \frac{c^2 h^2}{4} \frac{1 + \cos mh}{1 - \cos mh} \leq 0 \quad (2.33)$$

Solving this quadratic equation for $\epsilon$ yields:

$$\epsilon_1 = \frac{h^2}{4\tau \sin^2 \frac{mh}{2}} (1 - \sqrt{d}), \quad \epsilon_2 = \frac{h^2}{4\tau \sin^2 \frac{mh}{2}} (1 + \sqrt{d}) \quad (2.34)$$

since the viscosity $\epsilon$ is assumed to be a real number, we require that $d = 1 - (\frac{c}{h})^2 \sin^2 mh \geq 0$.

This requirement yields the following condition:

$$\left| \frac{c\tau}{h} \right| \leq 0 \quad (2.35)$$

where $\left| \frac{c\tau}{h} \right|$ is known as the CFL number and Equation 2.35 is called the CFL condition. Using $\epsilon_1$ and $\epsilon_2$, Equation 2.33 can be cast into the following form:

$$\left( \epsilon - \frac{h^2}{4\tau} \Gamma_1(mh) \right) \left( \epsilon - \frac{h^2}{4\tau} \Gamma_2(mh) \right) \leq 0 \quad (2.36)$$

where

$$\Gamma_1(mh) = \frac{(1 - \sqrt{d})}{\sin^2 \frac{mh}{2}}, \quad \Gamma_2(mh) = \frac{(1 + \sqrt{d})}{\sin^2 \frac{mh}{2}}$$

we need to analyze the behavior of functions $\Gamma_1$ and $\Gamma_2$ to obtain a more tangible stability criteria for $\epsilon$. Figure 4 shows plots of $\Gamma_1$ and $\Gamma_2$ for $0 \leq mh \leq 2\pi$ for a given CFL number, in
which it can be readily seen that the function $\Gamma_1$ is bounded from below and above while $\Gamma_2$ is only bounded from below. We also observe that $\Gamma_1 \leq \Gamma_2$, which necessitates the Equation 2.36 to be simplified to the following system of inequalities:

$$
\begin{align*}
    \epsilon - \frac{h^2}{4\tau} \Gamma_1(mh) &\geq 0 \\
    \epsilon - \frac{h^2}{4\tau} \Gamma_2(mh) &\leq 0
\end{align*}
$$

(2.37)

To find the solution of the right system of inequalities, we can use the diagram depicted in Figure 4 from which it is easily seen that the centered difference scheme is stable if it satisfies the following condition

$$
CFL \leq 1, \text{ and } \frac{h^2}{2\tau} CFL \leq \epsilon \leq \frac{h^2}{2\tau}
$$

(2.38)
It is more convenient to determine the viscosity coefficient $\epsilon$ as follows

$$\epsilon = C_{max} h \left| f'(u) \right| = C_{max} h |c|$$  \hspace{1cm} (2.39)

Recalling the fact that $|c|$ is the propagation speed and combining Equation 2.40 and Equation 2.37, we may present a new stability condition for $C_{max}$

$$CFL \leq 1, \quad \epsilon = C_{max} h |c| \quad \frac{CFL}{2} \leq C_{max} \leq \frac{1}{2CFL}$$ \hspace{1cm} (2.40)

From the above equation it can be observed that the viscosity $\epsilon$ vanishes as $h \to 0$. Therefore, it is sometimes referred to as the first order artificial viscosity. It is also noteworthy to note that the unperturbed or original conservation equation can be obtained by setting $\epsilon = 0$ and one can immediately conclude from above analysis that the centered difference scheme is unconditionally unstable since $0 < \frac{CFL}{2} h |c|$. This is a remarkable conclusion and implicates the need for some sort of artificial dissipation in numerical algorithms designed for solving conservation laws with discontinuous solutions. It is needless to say that this dissipation is solely needed in the vicinity of the discontinuity and should preferably vanishes as the grid spacing $h$ approaches zero.
2.2.2 Entropy-based Artificial Viscosity for Conservation Laws

In this section we construct the foundation of our numerical algorithm for adding dissipation to discontinuous flows in order to solve them in an accurate and stable fashion. As discussed above, the dissipation is added artificially to the governing equation in order to convert it from its original form into a perturbed or regularized form which leads to a viscosity vanishing solution. Thus, an artificial dissipation needs to be added to the equation which, as mentioned in the previous section, is preferably assumed to be large at shocks and goes smoothly to zero in the smooth regions of the solution. In Sec. 2.1 the behavior of entropy inequality was discussed for scalar one-dimensional conservation laws and it was observed that the aforementioned equation has a non-zero residual at shocks and turns into a conservation law for entropy in areas with smooth solution. We can take advantage of this property of entropy transport equation and use this entropy residual to construct a dissipation term which will inherently have the same behavior as the entropy residual which is favored in this context. To maintain the stability of the numerical solution, the entropy viscosity should be bounded by the first-order artificial viscosity from above. Since the residual of an entropy equation is supposed to be vanishingly small - of the order of the Local Truncation Error (LTE) in smooth regions and arbitrarily large in shocks, the entropy viscosity is almost zero everywhere except in shocks, where it reaches the first-order upper bound. The entropy viscosity method can be constructed in a few steps;
first we define an entropy residual for a given entropy pair \((\eta(u), \phi(u))\) based on the entropy inequality equation [Equation 2.23]

\[
D_h = \partial_t \eta(u) + \nabla \cdot \phi(u)
\] 

(2.41)

then we use the residual to define a viscosity, \(\epsilon_E\):

\[
\epsilon_E = C_E R_+ \frac{h^2}{\|\eta(u) - \overline{\eta(u)}\|_\infty}
\] 

(2.42)

where \(C_E\) is a tunable constant, \(R_+\) is a positive functional that remains to be specified, \(\|\|_\infty\) is an infinity norm and \(\eta(u)\) is the space averaged entropy. The \(R_+\) is supposed to remain positive throughout the domain to avoid having a negative viscosity and since \(D_h\) is expected to oscillate specially at shocks where it approximates a Dirac measure we set \(R_+ = |D_h|\) to avoid negative values. Introducing the scaling coefficient \(h^2\) along with the infinity norm of entropy, gives \(\epsilon_E\) the dimension of viscosity. Considering the Von Nuemann analysis conclusions, we might need to introduce an upper bound for the viscosity, say \(\epsilon_{\text{max}}\), to ensure the scheme’s stability

\[
\epsilon_{\text{max}} = C_{\text{max}} h \max |f'(u)|
\] 

(2.43)

and the artificial viscosity, which is called *entropy viscosity* hereafter, can naturally be formulated as:

\[
\epsilon = \max(\epsilon_E, \epsilon_{\text{max}})
\] 

(2.44)
In order to further describe the entropy viscosity method, we have to specify the numerical discretization which will be covered in Chapter 5. However, in the rest of this chapter we will demonstrate the capability of the entropy viscosity method in solving conservation laws with discontinuities through showing two examples in one space dimension.

### 2.2.3 One-dimensional Transport Equation

In this section we illustrate the performance of the entropy viscosity method in dealing with flow discontinuities. We consider two model problems in the context of one-dimensional conservation laws, namely, linear advection and inviscid Burgers equations. The former is a nonlinear equation and thus performs as a more rigorous test for the numerical scheme. The problems are solved subject to different initial conditions ranging from smooth waves to extremely sharp waves to observe how the code handles different type of initial conditions.

Consider the linear advection equation

$$\partial_t u + \partial_x u = 0, \quad 0 \leq x \leq 1 \tag{2.45}$$

with periodic boundary condition. The problem is exposed to three different types of initial conditions, namely sine wave, Gaussian exponential wave and square wave. We consider these three waves as three different levels of smoothness of initial disturbance. The simulations have been conducted within a domain with twenty $P^8$ elements, where $P$ indicates the order of the approximation polynomial within each element. The results are depicted in Figure 5 and Figure 6 for different types of initial conditions. In Figure 5(a), the solution without
using entropy viscosity is depicted in comparison with the exact solution for a sinusoidal initial condition. As it is clearly shown, the unaltered DSEM method is able to generate a solution with a good agreement to exact solution. For this smooth initial condition, there are no oscillations in the results after 20 time units. We can also use this case to assess the numerical diffusion introduced by the entropy viscosity method using the results displayed in Figure 5(b). Applying EV damps the amplitude of the wave by about 5% and this may be interpreted as a measure of the diffusion error.

As a more rigorous test case, we have combined a Gaussian exponential wave and a square wave to analyze the stability and accuracy of the method in comparison to the results obtained after using entropy viscosity. Figure 6(a) shows a comparison between the exact solution and the unaltered dG results. As seen from the figure, after 5 time units relatively large oscillations appear on top and around the square. It is clear that the unaltered method is not capable of handling abrupt discontinuities in the solution and we would need some remedy to overcome this problem. In Figure 6(b) the results after applying EV are shown. We can clearly see that EV is able to damp the oscillations and smoothen the solution without incurring a significant loss of accuracy.

It is important to mentions that using a residual to construct a viscosity is not a new idea. For example, the residual of the conservation equation itself can be employed, see [39,42]. Although the residual of the conservation equation is a good error indicator, it is far less robust than the entropy residual. The reason is that consistency requires the equation residual
vanishes as a grid size $h$ goes to zero, whereas the entropy residual converges to a Dirac measure supported in shocks.

Figure 5: Solutions for sine wave in linear advection equation in a domain with 20 $P8$ elements at $t=20$: (a) Unaltered DSEM, (b) DSEM with entropy viscosity.
Figure 6: Solutions for combination of square and exponential waves in linear advection equation in a domain with 20 $P^8$ elements at $t=5$: (a) Unaltered DSEM, (b) DSEM with entropy viscosity.
In this chapter we consider conservation laws of hyperbolic type which are the fundamental governing equations of fluid dynamics known as Navier-Stokes equations. Conservation laws arise from fundamental physical principles; conservation of mass, momentum and energy which will form the basis of discretized equations in the numerical scheme. In the first section, these conservation laws are derived in integral and differential forms. In the second part of this chapter, we derive the definition of entropy and its transport equation based on the second law of thermodynamics which will play an important role in the central idea of the shock capturing method used in this research effort.

3.1 Compressible Navier-Stokes Equations

3.1.1 Integral and Differential Forms

We begin by deriving the equation for conservation of mass in its integral form. Let $\Omega$ be an arbitrarily chosen connected domain with the boundary $S$, whose normal in every point is indicated with $n$, as depicted in Figure 7. The total mass within $\Omega$ is defined as the integral of the density:

$$m_\Omega = \int_\Omega \rho \, d\Omega.$$  \hspace{1cm} (3.1)

We assume that mass is neither created nor destroyed, then the mass in $\Omega$ can change only because of the mass flow across the boundary $S$. Applying the conservation of mass to an
Figure 7: Schematic representation of a generic control volume $\Omega$, boundary $S$ and its normal $\mathbf{n}$, immersed in a flow with velocity $\mathbf{u}$

infinitesimal surface element $dS$ and its normal $\mathbf{n}$ and extending it over the whole domain, we can obtain the integral form of the mass conservation law:

$$
\int_{\Omega} \frac{\partial \rho}{\partial t} \, d\Omega + \int_{S} \rho \mathbf{u} \cdot \mathbf{n} \, dS = 0.
$$

(3.2)

The surface integral can be transformed into a volume integral by applying Gauss divergence theorem, and brought for convenience to the left hand side.

$$
\int_{\Omega} \left[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) \right] \, d\Omega = 0.
$$

(3.3)
Another integral form of the same conservation law is obtained by integrating Equation 3.3 in time from any $t_1$ to any $t_2 > t_1$:

$$\int_{t_1}^{t_2} \int_{\Omega} \left[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) \right] \, d\Omega = 0.$$  \hspace{1cm} (3.4)

Since the domain $\Omega$ and time $t$ are arbitrarily chosen, one may conclude that the integrand in Equation 3.4 must be identically zero for all $\mathbf{x} \in \Omega$ and $t$:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0.$$  \hspace{1cm} (3.5)

which is the desired differential form of the mass conservation law. Equation 3.5 must be typically solved in conjunction with the equations for conservation of momentum and total energy. By following a procedure similar to the former, an expression for the momentum conservation in integral form can be derived:

$$\frac{\partial}{\partial t} \int_{\Omega} \rho \mathbf{u} \, d\Omega + \int_{S} (\rho \mathbf{u} \otimes \mathbf{u}) \cdot \mathbf{n} \, dS = - \int_{S} p \mathbf{I} \cdot \mathbf{n} \, dS + \int_{S} \tau \cdot \mathbf{n} \, dS.$$  \hspace{1cm} (3.6)

where, $\tau$, represents the viscous stress tensor

$$\tau = \mu (2 \mathbf{S}) + \left( \beta - \frac{2}{3} \mu \right) (\nabla \cdot \mathbf{u}) \mathbf{h}.$$  \hspace{1cm} (3.7)
where \( \mu \) is the dynamic viscosity; \( \beta \) is the bulk viscosity and \( S \) is the strain rate tensor,

\[
S = \frac{1}{2} \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right]
\] (3.8)

in this work the physical bulk viscosity of the fluid is taken to be zero following the Stokes hypothesis. Applying the mass conservation equation and Gauss divergence theorem, Equation 3.6 can be rewritten in differential form

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \tau.
\] (3.9)

The third fundamental equation of fluid dynamics states the conservation of total energy, given by the sum of kinetic, potential and internal energy. The integral form of energy conservation law can be formulated as:

\[
\frac{\partial}{\partial t} \int_\Omega \rho e_t \, d\Omega = -\int_S \rho e_t \mathbf{u} \cdot \mathbf{n} \, dS - \int_S \mathbf{q}_\alpha \cdot \mathbf{n} \, dS - \int_S (p \mathbf{I} - \tau) \cdot \mathbf{u} \, dS.
\] (3.10)

where, \( e_t \) is the total energy per unit volume and \( \mathbf{q}_\alpha \) is the thermal flux. Following the same routine and considering the same assumption as in the momentum equation, the equivalent differential form for energy conservation can be expressed as

\[
\frac{\partial (\rho e_t)}{\partial t} + \nabla \cdot (\rho e_t \mathbf{u}) = -\nabla \cdot (p \mathbf{u}) - \nabla \cdot \mathbf{q}_\alpha + \nabla \cdot \tau.
\] (3.11)

which is the final conservation equation for total energy.
3.1.2 Non-dimensional Form

The differential form of compressible Navier-Stokes equations derived in the previous section, can be cast into the following form for a Newtonian and continuous fluid:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{3.12}
\]

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{uu} + p\delta) - \nabla \cdot \mathbf{T} = 0 \tag{3.13}
\]

\[
\frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho e \mathbf{u} + p\delta \cdot \mathbf{u}) - \nabla \cdot (\mathbf{T} \cdot \mathbf{u} + \kappa \nabla T) = 0 \tag{3.14}
\]

where \( \delta \) is the Kronecker tensor. It is assumed that the thermal flux can be expressed using Fourier's law as

\[
\mathbf{q}_\alpha = -\lambda \nabla T = -\rho c_p \alpha \nabla T,
\]

where \( \kappa \) is the thermal conductivity \([W/(mK)]\), while \( \alpha \) is the thermal diffusivity \([m^2/s]\), linked by the relation \( \alpha = \kappa / (\rho c_p) \). The governing equations can be non-dimensionalized by using non-dimesnionalized variables:

\[
\begin{align*}
\tilde{x} &= \frac{x}{l_f}, & \tilde{y} &= \frac{y}{l_f}, & \tilde{z} &= \frac{z}{l_f}, \\
\tilde{u} &= \frac{u}{v_f}, & \tilde{v} &= \frac{v}{v_f}, & \tilde{w} &= \frac{w}{v_f}, \\
\tilde{\rho} &= \frac{\rho}{\rho_f}, & \tilde{T} &= \frac{T}{T_f}, & \tilde{p} &= \frac{p}{\rho_f v_f^2}, \\
\tilde{t} &= \frac{tv_f}{l_f},
\end{align*}
\]
and introducing non-dimensional group parameters: Reynolds number, $Re_f$, Prandtl number, $Pr_f$, and Mach number, $M_f$ as

$$Re_f = \frac{U_f L_f \rho_f}{\mu}, \quad Pr_f = \frac{c_p \mu}{\kappa}, \quad M_f = \frac{U_f}{\sqrt{\gamma RT_f}}$$

where ˇ denotes a non-dimensional variable; subscript $f$ denotes the reference scale; $c_p$ is the constant-pressure specific heat; $R$ is the gas constant and $\gamma$ is the ratio of specific heats. Using these parameters, and assuming constant fluid properties, the non-dimensional form of (Equation 3.12) - (Equation 3.14) reads,

$$\frac{\partial \hat{\rho}}{\partial \hat{t}} + \nabla \cdot (\hat{\rho} \hat{u}) = 0 \tag{3.15}$$

$$\frac{\partial (\hat{\rho} \hat{u})}{\partial \hat{t}} + \nabla \cdot (\hat{\rho} \hat{u} \hat{u} + \hat{p} \delta) - \frac{1}{Re_f} \nabla \cdot \tau = 0 \tag{3.16}$$

$$\frac{\partial (\hat{\rho} \hat{e})}{\partial \hat{t}} + \nabla \cdot (\hat{\rho} \hat{e} \hat{u} + \hat{p} \delta \cdot \hat{u}) - \frac{1}{Re_f} \nabla \cdot \left( \tau \cdot \hat{u} + \frac{\kappa}{(\gamma - 1) M_f^2 Pr_f} \nabla T \right) = 0 \tag{3.17}$$

From this point onward we drop the accent ˇ for simplicity. (Equation 3.15) - (Equation 3.17) count for five equations while there are six unknowns $\rho, u, v, w, p$ and $T$. It means that we need to close the systems with an appropriate equation, which is called the Equation of State (EoS) and links the pressure with other unknowns. There is an abundant number of equations
of state that are presently available to describe compressible fluids; however, in the present work we utilize the simplest possible model of a compressible fluid called an ideal gas EoS.

\[ p = \rho RT, \quad (3.18) \]

where \( R \left[ \text{J}/(\text{KgK}) \right] \) is the gas constant. The ideal gas equation of state in non-dimensional form is given by \( p = \frac{\rho T}{\gamma M_f} \).

Now that all the fundamental equations have been presented in their non-dimensional forms, it is convenient to group them into a matrix form, that is the most suitable for a CFD application. Therefore, all conservation equations may be reunited under the following relation:

\[
\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{F}_f}{\partial x} + \frac{\partial \mathbf{G}_f}{\partial y} + \frac{\partial \mathbf{H}_f}{\partial z} = \frac{1}{Re_f} \left[ \left( \frac{\partial \mathbf{F}_\nu}{\partial x} + \frac{\partial \mathbf{G}_\nu}{\partial y} + \frac{\partial \mathbf{H}_\nu}{\partial z} \right) + \left( \frac{\partial \mathbf{F}_T}{\partial x} + \frac{\partial \mathbf{G}_T}{\partial y} + \frac{\partial \mathbf{H}_T}{\partial z} \right) \right]. \quad (3.19)
\]

Vectors constituting Equation 3.19 can be subdivided in

- Vector of conserved quantities, \( \mathbf{q} \)

\[
\mathbf{q} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho e_t \end{pmatrix}; \quad (3.20)
\]
Vectors that group inviscid (advection and hydrostatic) fluxes along the Cartesian coordinates, \( \mathbf{F}_f, \mathbf{G}_f \) and \( \mathbf{H}_f \):

\[
\mathbf{F}_f = \begin{pmatrix}
\rho u \\
\rho u^2 + p \\
\rho u v \\
\rho w \\
(\rho e_t u + pu)
\end{pmatrix}, \quad \mathbf{G}_f = \begin{pmatrix}
\rho v \\
\rho v^2 + p \\
\rho v w \\
\rho w \\
(\rho e_t v + pw)
\end{pmatrix}, \quad \mathbf{H}_f = \begin{pmatrix}
\rho w \\
\rho w v \\
\rho w^2 + p \\
(\rho e_t w + pw)
\end{pmatrix};
\]

Vectors that group viscous fluxes along the Cartesian coordinates, \( \mathbf{F}_\nu, \mathbf{G}_\nu \) and \( \mathbf{H}_\nu \):

\[
\mathbf{F}_\nu = \begin{pmatrix}
0 \\
\tau_{xx} \\
\tau_{xy} \\
\tau_{xz} \\
(ut_{xx} + v t_{xy} + w t_{xz})
\end{pmatrix}, \quad \mathbf{G}_\nu = \begin{pmatrix}
0 \\
\tau_{xy} \\
\tau_{yy} \\
\tau_{yz} \\
(ut_{xy} + v t_{yy} + w t_{yz})
\end{pmatrix};
\]

\[
\mathbf{H}_\nu = \begin{pmatrix}
0 \\
\tau_{xz} \\
\tau_{yz} \\
\tau_{zz} \\
(ut_{xz} + v t_{yz} + w t_{zz})
\end{pmatrix}.
\]
• Vectors that group the influence of temperature, \(F_T, G_T, H_T\)

\[
F_T = \begin{pmatrix}
0 \\
0 \\
0 \\
\frac{1}{(\gamma-1)M_f^2 Pr} \frac{\partial T}{\partial x}
\end{pmatrix}, \quad G_T = \begin{pmatrix}
0 \\
0 \\
0 \\
\frac{1}{(\gamma-1)M_f^2 Pr} \frac{\partial T}{\partial y}
\end{pmatrix}, \quad H_T = \begin{pmatrix}
0 \\
0 \\
0 \\
\frac{1}{(\gamma-1)M_f^2 Pr} \frac{\partial T}{\partial z}
\end{pmatrix}.
\]

The components \(\tau_{ij}\) of the stress tensor are here defined as

\[
\tau_{xx} = 2 \left( \frac{\partial u}{\partial x} - \frac{1}{3} \nabla \cdot \mathbf{v} \right),
\]
\[
\tau_{yy} = 2 \left( \frac{\partial v}{\partial y} - \frac{1}{3} \nabla \cdot \mathbf{v} \right),
\]
\[
\tau_{zz} = 2 \left( \frac{\partial w}{\partial z} - \frac{1}{3} \nabla \cdot \mathbf{v} \right),
\]
\[
\tau_{xy} = \tau_{yx} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x},
\]
\[
\tau_{yz} = \tau_{zy} = \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y},
\]
\[
\tau_{xz} = \tau_{zx} = \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z}.
\]

To solve the above system of equations, the initial data \(q_0\) is supposed to be known. If the equations have to be solved on some bounded domain, then we also need to include the appropriate types of boundary conditions, such as inflow or outflow boundaries, slip or no-slip boundaries, and others.
### 3.2 Entropy Generation and Transport Equations

In this section we present some rigorous analysis about the entropy of a system and present mathematical relations which state how the entropy of a fluid is affected by its motion. We begin by considering the Gibbs equation on a fluid element

\[ \rho \frac{De}{Dt} - \left( \frac{p}{\rho} \right) \frac{D\rho}{Dt} = \rho T \frac{Ds}{Dt} \]  
\[ (3.21) \]

where, \( s \) is the fluids entropy. For an ideal, calrorically perfect gas we can write the difference in fluid’s entropy between two hypothetical states as:

\[ s_2 - s_1 = c_v \ln \left[ \frac{\rho_2}{\rho_1} \left( \frac{\rho_1}{\rho_2} \right)^\gamma \right] \]
\[ (3.22) \]

which gives the following expression for entropy with respect to a reference state:

\[ s = c_v \ln \left[ \frac{p}{\rho^\gamma} \right] \]
\[ (3.23) \]

Now, let’s look at the internal energy conservation equation in terms of substantial derivative:

\[ \rho \frac{De}{Dt} + p \nabla \cdot \mathbf{u} = -\nabla \cdot \mathbf{q}_T + \nabla \cdot (\mathbf{z} \cdot \mathbf{u}) \]
\[ (3.24) \]
where \( \mathbf{q}_T \) is the vector of heat flux. We can also write the continuity equation in terms of substantial derivatives as:

\[
\left( \frac{p}{\rho} \right) \frac{D\rho}{Dt} = -p \nabla \cdot \mathbf{u}.
\] (3.25)

Now, by substituting the continuity equation (3.15) in the energy equation (3.24), we obtain a new form of the energy equation:

\[
\rho \frac{De}{Dt} - \left( \frac{P}{\rho} \right) \frac{D\rho}{Dt} = -\nabla \cdot \mathbf{q}_T + \nabla \cdot (\tau \cdot \mathbf{u})
\] (3.26)

Comparing this form of the energy equation with the Gibbs equation, we see that the left-hand-side corresponds to the entropy term

\[
\rho T \frac{Ds}{Dt} = -\nabla \cdot \mathbf{q}_T + \nabla \cdot (\tau \cdot \mathbf{u}).
\] (3.27)

By using the continuity equation one more time we can convert Equation 3.29 into a conservation equation for entropy:

\[
\rho \frac{\partial s}{\partial t} + \rho \mathbf{u} \cdot \nabla s = -\nabla \cdot \mathbf{q}_T + \nabla \cdot (\tau \cdot \mathbf{u}) \quad \frac{T}{T}.
\] (3.28)

\[
s \frac{\partial \rho}{\partial t} + s \mathbf{u} \cdot \nabla \rho + s \rho \nabla \cdot \mathbf{u} = 0.
\] (3.29)

Adding these two equations to each other we get:

\[
\frac{\partial \rho s}{\partial t} + \nabla \cdot (\mathbf{u} \rho s) = -\frac{\nabla \cdot \mathbf{q}_T}{T} + \frac{\nabla \cdot (\tau \cdot \mathbf{u})}{T}.
\] (3.30)
The heat flux term can be rearranged into a divergence term and a squared term as:

$$\nabla \cdot \left( \frac{q_T T}{T} \right) = \nabla \cdot q_T - \frac{q_T^2}{T^2} \nabla T. \quad (3.31)$$

the heat flux term can be formulated in terms of the thermal conductivity and temperature gradient:

$$q_T = -\kappa \nabla T \quad (3.32)$$

by substituting Equation 3.31 and Equation 3.32 in entropy transport equation, we can cast this equation into a new form:

$$\frac{\partial \rho s}{\partial t} + \nabla \cdot \left( \rho s \mathbf{u} - \kappa \nabla T \right) = \nabla \cdot \left( \frac{\mathbf{\tau} \cdot \mathbf{u}}{T} \right) + \frac{\kappa (\nabla T)^2}{T^2}. \quad (3.33)$$

Now let

$$\Phi = \nabla \cdot (\mathbf{\tau} \cdot \mathbf{u}), \quad \Gamma = \frac{\kappa (\nabla T)^2}{T}, \quad \Lambda = \nabla \cdot \left( \frac{\kappa}{T} \nabla T \right).$$

The scalar quantity, $\Phi$, is the viscous dissipation of kinetic energy which appears as a generation term in entropy transport equation due to irreversible conversion of kinetic energy to internal energy due to viscous friction. Similarly, $\Gamma$ is the entropy generation due to thermal
irreversibilities and Λ denotes the transport of entropy due to diffusion. Now, the final form of entropy transport equation can be expressed as

$$\frac{D \rho s}{Dt} = \frac{\Phi + \Gamma}{T} + \Lambda$$  \hspace{1cm} (3.34)

In order to convert this equation into a non-dimensional form, we need to introduce the non-dimensional entropy. Recalling the second law of thermodynamics can lead us to a proper reference scale for entropy:

$$\tilde{s} = \frac{s}{v_f^2/T_f}$$  \hspace{1cm} (3.35)

by substituting in [Equation 3.23] and after some simplifications, the non-dimensional definition of entropy may be represented as:

$$\tilde{s} = \frac{1}{\gamma(\gamma - 1)} \ln \left[ \frac{\tilde{\rho}}{\tilde{\rho}^\gamma} \right]$$  \hspace{1cm} (3.36)

By using the non-dimensional forms of entropy and other independent variables defined in the previous sections, [Equation 3.34] can be expressed in a non-dimensional form:

$$\frac{D \tilde{\rho}\tilde{s}}{Dt} = \frac{1}{Re_f \tilde{T}} \frac{\tilde{\Phi}}{T} + \frac{1}{Pr_f Re_f(\gamma - 1)M_f^2 \tilde{T}} \frac{\tilde{\Gamma}}{T} + \frac{1}{Pr_f Re_f(\gamma - 1)M_f^2 \tilde{T}} \Lambda$$  \hspace{1cm} (3.37)
again, \( \ddot{\cdot} \) denotes a non-dimensional variable. For simplicity, hereinafter we drop this accent. In a Cartesian coordinates system and assuming zero bulk viscosity, \( \Phi, \Gamma \) and \( \Lambda \) are defined by the following relations:

\[
\Phi = 2 \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 + \left( \frac{\partial w}{\partial z} \right)^2 \right] + \left[ \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)^2 \right] - \frac{2}{3} \left[ \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)^2 \right],
\]

\[
\Gamma = \left[ \left( \frac{\partial T}{\partial x} \right)^2 + \left( \frac{\partial T}{\partial y} \right)^2 + \left( \frac{\partial T}{\partial z} \right)^2 \right],
\]

\[
\Lambda = \left[ \frac{\partial}{\partial x} \left( \frac{1}{T} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{1}{T} \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( \frac{1}{T} \frac{\partial T}{\partial z} \right) \right].
\]

It should be remarked that, the first two terms on the right hand side of the entropy transport equation are always positive and can be considered as the entropy source terms. This result provides an explicit expression for the irreversible changes in entropy that occur in a compressible flow when all the field are smooth. But when dealing with shocked flows, entropy transport equation does not describe the behavior of the system. It has been shown, see for example [45], that the entropy of a fluid particle can increase or jump to a higher value when the particle passes a shock. In this case the entropy transport equation should be written as an inequality:

\[
\frac{D\rho s}{Dt} - \left[ \frac{1}{Re_f T} + \frac{1}{Pr_f Re_f (\gamma - 1) M_f^2 T} + \frac{1}{Pr_f Re_f (\gamma - 1) M_f^2} \Lambda \right] > 0 \quad (3.38)
\]
As it will be seen in Chapters 4 and 5, this inequality plays a crucial role in further discussion of numerical schemes which are based on the entropy production in the interior of shock waves. Before closing this chapter, we would like to bring our attention to the special case of Euler equations and briefly present the entropy transport equation for gas dynamics problems, governed by the Euler system of Equations. For inviscid flows, both the dynamic and bulk viscosity coefficients as well as the thermal conduction coefficient are zero.
CHAPTER 4

DISCONTINUOUS SPECTRAL ELEMENT METHOD ON STAGGERED GRID

To discretize the governing equations derived in the previous chapter we use a nodal collocation form of the discontinuous spectral element method (DSEM) \cite{1, 2, 49, 50}. For time integration, a fourth-order, low-storage Runge-Kutta method is used \cite{51}. Below, we describe the implementation of the DSEM in three dimensions.

In DSEM the approximation begins with the subdivision of the domain into multiple subdomains, called elements, where the spectral approximation is applied. These elements are non-overlapping which allows the governing equation to be solved locally inside each subdomain. The local nature of this method enables meshing of complex flow geometries and ensure a high parallel efficiency and easy boundary condition implementation. In three space dimensions, the domain, \( \Omega \), is divided into elements

\[
\Omega = \sum_k \Omega_k, \; k = 0, 1, \ldots, K. \tag{4.1}
\]

where \( \Omega_k \) is the \( k \)-th element.

In DSEM the approximation process involves using the Chebyshev polynomial to approximate the solution. These polynomials are defined on the interval of \([0, 1]\) and therefore, to use this polynomial on generic subdomain \( \Omega_k \) it is necessary to map the domain to the same interval.
in all spatial dimensions. The mapping process maps each curved element in three dimensional physical space with any arbitrary shape to a unit cube in the computational domain. This operation is performed using isoparametric mapping which ensures that the spectral accuracy of the scheme is not affected by the domain boundary approximation.

4.1 Isoparametric Mapping

To perform the mapping process, we should constitute proper instruments for transforming corners, curves and surfaces from the physical domain to the computational domain. The parametric curve $g(s)$, with $0 \leq s \leq 1$, is interpolated by the polynomial $P(s)$, which has the same degree as the approximation order within the domain. In particular, the interpolating polynomial $P$ is defined as a linear combination of the fundamental polynomials

$$P(s) = \sum_{j=0}^{N} g_j l_j(s), \quad (4.2)$$

where $l_j(s)$ are the fundamental Lagrangian polynomials, which constitute a base of the polynomials space, and are given by

$$l_j(s) = \prod_{i=0, i \neq j}^{N} \frac{s - x_i}{x_j - x_i}. \quad (4.3)$$

Similarly, the parametric surface we introduce the interpolating polynomial $S$ which interpolates the boundary surface $g(s,t)$, with $0 \leq s,t \leq 1$, is interpolated by the polynomial $S(s,t)$

$$S(s,t) = \sum_{i=0}^{N} \sum_{j=0}^{N} g_{ij} l_i(s) l_j(t), \quad (4.4)$$
The three dimensional mapping is then performed using the linear blending formula [52]

\[
x(X, Y, Z) = (1 - Y)S_1(X, Z) + YS_2(X, Z) + (1 - Z)S_3(X, Y) + \\
+ XS_4(Y, Z) + ZS_5(X, Y) + (1 - X)S_6(Y, Z) + \\
- (1 - Y)(1 - Z)P_1(X) - X(1 - Y)P_2(Z) - (1 - Y)ZP_3(X) + \\
- (1 - X)(1 - Y)P_4(Z) - Y(1 - Z)P_5(X) - XYP_6(Z) + \\
- YZP_7(X) - (1 - X)YP_8(Z) - (1 - X)(1 - Z)P_9(Y) + \\
- X(1 - Z)P_{10}(Y) - XZP_{11}(Y) - (1 - X)ZP_{12}(Y) + \\
+ (1 - X)(1 - Y)(1 - Z)x_1 + X(1 - Y)(1 - Z)x_2 + XY(1 - Z)x_3 + \\
+ (1 - X)Y(1 - Z)x_4 + (1 - X)(1 - Y)Zx_5 + X(1 - Y)(1 - Z)x_6 + \\
+ XYZx_7 + (1 - X)YZx_8.
\]

Equations for \(y(X, Y, Z)\) and \(z(X, Y, Z)\) can be obtained directly from Equation 4.5 replacing \(x_i\) on the right-hand side with \(y_i\) or \(z_i\) respectively, therefore their formulation is omitted here.

A graphical representation of the elements’ numbering is shown in Figure 8, where the left representation shows the top, front, and right face numbering, while the right representation highlights the bottom, right and rear faces. The bigger font has been used to indicate the faces’ numbers, while the sides have been indicated with smaller italic numbers, and corners’ numbering is underlined and overlined [53].
4.1.1 Mapped Equations

Using the mapping operator presented in the previous section, the general form of governing equations becomes:

\[
\frac{\partial \tilde{q}}{\partial t} + \frac{\partial \tilde{F}}{\partial X} + \frac{\partial \tilde{G}}{\partial Y} + \frac{\partial \tilde{H}}{\partial Z} = 0,
\]

(4.6)

where \( \tilde{q} \) indicates the mapped vector of conservative variables and \( \tilde{F}, \tilde{G} \) and \( \tilde{H} \) indicate the mapped vector of fluxes in \( X, Y \) and \( Z \) directions, respectively. The solution values in the mapped space are related to their values in physical space as:

\[
\tilde{q} = Jq.
\]

(4.7)
where $J$ is the determinant of the Jacobian matrix of the coordinate transformation which can be expressed as

$$
J(x, y, z) = \frac{\partial x}{\partial X} \left( \frac{\partial y}{\partial Y} \frac{\partial z}{\partial Z} - \frac{\partial y}{\partial Z} \frac{\partial z}{\partial Y} \right) - \frac{\partial x}{\partial Y} \left( \frac{\partial y}{\partial X} \frac{\partial z}{\partial Z} - \frac{\partial y}{\partial Z} \frac{\partial z}{\partial X} \right) + \frac{\partial x}{\partial Z} \left( \frac{\partial y}{\partial X} \frac{\partial z}{\partial Y} - \frac{\partial y}{\partial Y} \frac{\partial z}{\partial X} \right).
$$

Similarly, the flux vectors in the mapped space can be expresses in terms of their counterparts in the physical space:

$$
\tilde{\mathbf{F}} = \frac{\partial X}{\partial x} \mathbf{F} + \frac{\partial X}{\partial y} \mathbf{G} + \frac{\partial X}{\partial z} \mathbf{H},
$$

$$
\tilde{\mathbf{G}} = \frac{\partial Y}{\partial x} \mathbf{F} + \frac{\partial Y}{\partial y} \mathbf{G} + \frac{\partial Y}{\partial z} \mathbf{H},
$$

$$
\tilde{\mathbf{H}} = \frac{\partial Z}{\partial x} \mathbf{F} + \frac{\partial Z}{\partial y} \mathbf{G} + \frac{\partial Z}{\partial z} \mathbf{H}.
$$

### 4.1.2 Staggered-Grid Spectral Method

In the following, a staggered-grid spectral method is described in detail. The DSEM method uses a staggered grid, namely two sets of grid, one for solution which are the Gauss quadrature nodes, and another set for computation of fluxes which are the Lobatto quadrature nodes. We first describe the space discretization in one-dimension for its simplicity and the extension to three dimensions should follow naturally. In one space dimension the Gauss points are defined as roots of Chebyshev polynomial of degree $n + 1$:

$$
X_{j+1/2} = \frac{1}{2} \left[ \cos \left( \frac{(2j + 1)\pi}{2n} \right) \right] \quad j = 0, ..., n - 1.
$$
and similarly the Gauss-Lobatto grid points are the roots of Chebyshev polynomials of degree $n$, given by:

$$X_j = \frac{1}{2} \left[ \cos \left( \frac{j \pi}{n} \right) \right] \quad j = 0, \ldots, n. \quad (4.13)$$

It should be underlined that, these points are defined on the unit interval $[0,1]$. In addition, while all Gauss points lie inside the interval considered, i.e. if the interval considered is $[a,b]$, Gauss points are such that $a < x_i < b$, whereas Lobatto points include also the two endpoints, which means Lobatto points obey the condition $a \leq x_i \leq b$. As it stems from the above equations, each Gauss point lies between two consecutive Gauss-Lobatto points, but not necessarily half way between them. A graphic representation of Gauss and Gauss-Lobatto points is depicted in Figure 9.

![Figure 9: One-dimensional representation of Lobatto and Gauss grids. The filled circles represent Gauss points, while the open circles represent Lobatto points.](image-url)
Now we can formulate the representation of solution values and fluxes on Gauss and Gauss-Lobatto grids, respectively. The approximation of \( \tilde{q} \) can be shown as:

\[
\tilde{q}^g(X) = \sum_{i=0}^{n-1} \tilde{q}_i^g h_{i+1/2}(X), \tag{4.14}
\]

where superscript ‘\( g \)’ indicates the grid considered is the Gauss grid, and \( h_{i+1/2} \) is the Lagrange interpolating polynomial on Gauss grid of degree \( n - 1 \), given by

\[
h_{i+1/2}(s) = \prod_{j=0, i \neq j}^{n-1} \frac{s - X_{j+1/2}}{X_{i+1/2} - X_{j+1/2}}. \tag{4.15}
\]

A similar formulation pertaining to fluxes \( F \) can be framed on the Lobatto grid:

\[
F^l(X) = \sum_{i=0}^{n} F_i^l l_i(X), \tag{4.16}
\]

with the Lagrangian interpolating polynomial of degree \( n \), \( l_i(X) \), expressed as

\[
l_i(s) = \prod_{j=0, i \neq j}^{n} \frac{s - X_j}{X_i - X_j}. \tag{4.17}
\]

where the superscript ‘\( l \)’ indicates the use of Lobatto grid for the approximation of fluxes. Expanding the above formulation to three-dimension is straightforward and only needs some subtle adjustments because of the higher number of dimensions involved.
Figure 10: Representation of Lobatto and Gauss grids, three-dimensional representation with sectioning plane on the left, two-dimensional section on the right. The filled circles represent Gauss/Gauss/Gauss points (GGG), the open squares Lobatto/Gauss/Gauss points (LGG), the open triangles Gauss/Lobatto/Gauss points (GLG) and the open circles Gauss/Gauss/Lobatto points (GGL).

In three dimensions, we are dealing with a unit cube as our computational domain instead of the unit interval, and subsequently, we expect the Gauss and Gauss-Lobatto grids to extend in space. Figure 10 displays a schematic of the Gauss and Lobatto grids in three dimensions. The Gauss grid includes the Gauss/Gauss/Gauss (GGG) points, represented by coordinates
\((X_{i+1/2}, Y_{j+1/2}, Z_{k+1/2}), \ i, j, k = 0, ..., n - 1\). The solution values are approximated on these points in a similar fashion to what was presented for the 1D case:

\[
\tilde{q}^{ggg}(X, Y, Z) = \sum_{p=0}^{n-1} \sum_{q=0}^{n-1} \sum_{r=0}^{n-1} \tilde{q}^{ggg}_{p+1/2,q+1/2,r+1/2} h_{p+1/2}(X) h_{q+1/2}(Y) h_{r+1/2}(Z); \quad (4.18)
\]

where again, \(h\) is the Lagrange interpolating polynomial. The flux approximation in three dimensions is a bit more involved as we will have three different sets of Gauss-Lobatto points.

The first component of the flux tensor, \(\tilde{F}\), is approximated on the Lobatto-Gauss-Gauss (LGG) points, with coordinates \((X_i, Y_{j+1/2}, Z_{k+1/2})\), with \(i, j, k\) such that \(i = 0, ..., n\) and \(j, k = 0, ..., n - 1\). Similarly, \(\tilde{G}\) and \(\tilde{H}\) are approximated on the Gauss/Lobatto/Gauss points (GLG) and Gauss/Gauss/Lobatto points (GGL), respectively.

The next step towards forming the discretized governing equations for the Navier-Stokes system is to evaluate fluxes on the Gauss-Lobatto grids. Before the flux values can be computed at the Gauss-Lobatto points, the solution values should be interpolated from the GGG points to LLG, GLG and GGL points. This process is carried out through interpolations using polynomials of the type in (Equation 4.15). The interpolation operation is given as:

- For the \(X\) direction

\[
q^{gg}(X_i, Y_{j+1/2}, Z_{k+1/2}) = \sum_{p=0}^{n-1} q^{gg}_{p+1/2,q+1/2,r+1/2} h_{p+1/2}(X_i); \quad (4.19)
\]
• For the $Y$ direction

$$
q^{glg}(X_{i+1/2}, Y_j, Z_{k+1/2}) = \sum_{q=0}^{n-1} q^{ggg}_{p+1/2,q+1/2,r+1/2} h_{q+1/2}(Y_j);
$$

(4.20)

• For the $Z$ direction

$$
q^{ggl}(X_{i+1/2}, Y_{j+1/2}, Z_k) = \sum_{r=0}^{n-1} q^{ggg}_{p+1/2,q+1/2,r+1/2} h_{r+1/2}(Z_k).
$$

(4.21)

Once the solution values are interpolated on the Gauss-Lobatto points, the advective fluxes can be determined using their functional relations with the conservative variables inside each element. However, the flux values are different at the elements faces due to discontinuity of the solution values. In order to ensure consistency to the method used, the flux must be a continuous and differentiable function throughout the domain, and especially at the interface between two neighboring domains. This calls for some additional treatment of fluxes at the interfaces which is called “patching” of fluxes. The patching process is explained in detail in Sec. 4.1.3.

The viscous fluxes are constructed in a two-step process. Following Bassi and Rebay [54] computation of the viscous fluxes involves taking derivatives of the solutions re-constructed at the Lobatto grid, which calls for a continuous solution at the Lobatto/Gauss and Gauss/Lobatto points. To construct a continuous approximation, the average of the solution on either side of the interface is used as the interface value. The continuous solution is then used to calculate the derivatives needed for the viscous fluxes. Once the derivatives are calculated on the Gauss grid,
they will be interpolated one more time to the Gauss-Lobatto points. To construct a continuous approximation, the average of the viscous fluxes are used on either side of the interface as the interface value. The total fluxes in $X$, $Y$ and $Z$ directions are then determined by summing the advective and viscous parts. Once the total fluxes are computed on the Gauss-Lobatto grid, the flux interpolants are constructed as

$$
\tilde{F}(X, Y, Z) = \sum_{p=0}^{n} \sum_{q=0}^{n-1} \sum_{r=0}^{n-1} \tilde{F}_{l,q+1/2,r+1/2}^{g,q+1/2} l_p(X) h_{q+1/2}(Y) h_{r+1/2}(Z);
$$

$$
\tilde{G}(X, Y, Z) = \sum_{p=0}^{n-1} \sum_{q=0}^{n} \sum_{r=0}^{n-1} \tilde{G}_{p+1/2,q+1/2,r}^{g,q+1/2} h_{p+1/2}(X) l_q(Y) h_{r+1/2}(Z);
$$

$$
\tilde{H}(X, Y, Z) = \sum_{p=0}^{n-1} \sum_{q=0}^{n-1} \sum_{r=0}^{n} \tilde{H}_{p+1/2,q+1/2,r}^{g,q+1/2} h_{p+1/2}(X) h_{q+1/2}(Y) l_r(Z).
$$

The fluxes just obtained are then differentiated and calculated at the Gauss grid, with

$$
\frac{\partial \tilde{F}(X_{i+1/2}, Y_{j+1/2}, Z_{k+1/2})}{\partial X} = \sum_{p=0}^{n} \tilde{F}(X_p, Y_{j+1/2}, Z_{k+1/2}) \frac{\partial l_p(X_{i+1/2})}{\partial X};
$$

$$
\frac{\partial \tilde{G}(X_{i+1/2}, Y_{j+1/2}, Z_{k+1/2})}{\partial Y} = \sum_{q=0}^{n} \tilde{G}(X_{i+1/2}, Y_q, Z_{k+1/2}) \frac{\partial l_q(Y_{j+1/2})}{\partial Y};
$$

$$
\frac{\partial \tilde{H}(X_{i+1/2}, Y_{j+1/2}, Z_{k+1/2})}{\partial Z} = \sum_{r=0}^{n} \tilde{H}(X_{i+1/2}, Y_{j+1/2}, Z_r) \frac{\partial l_r(Z_{k+1/2})}{\partial Z}.
$$

The final semi-discrete equation at the Gauss grid is given by:

$$
\left[ \frac{d\tilde{q}}{dt} \right] + \left[ \frac{\partial \tilde{F}}{\partial X} \right] + \left[ \frac{\partial \tilde{G}}{\partial Y} \right] + \left[ \frac{\partial \tilde{H}}{\partial Z} \right] = 0, \quad (4.22)
$$
where each term is calculated on the Gauss grid \((i + 1/2, j + 1/2, k + 1/2)\), and which is then advanced in time with a 4-th order low storage Runge-Kutta scheme.

4.1.3 **Interface and Boundary Treatment**

As explained in the previous section, the interpolation of solution from the Gauss grid into the Lobatto grid leads to a discontinuity in solution at the element interfaces. Since constructing advective and viscous fluxes calls for a continuous and single-valued derivatives of the solution, its discontinuity at the interfaces can be troublesome. Therefore some special treatments are needed at the element interfaces.

The treatment performed on the advective and viscous fluxes at the interfaces is called patching. Patching enforces the fluxes to be continuous at the interfaces which is a necessary condition for a conservative method. In principle, patching includes two separate processes; a Dirichlet patching which ensures the uniqueness of the first derivative of solution, and a Neumann patching which ensures the uniqueness of the viscous flux derivative.

The patching process is carried out using a so-called mortar method. In this approach, the Gauss-Lobatto fluxes from each two neighboring elements which share an interface, are projected to a mortar where a unique flux is calculated which will be projected back to each side of the mortar and thus yielding a unique and continuous flux. In this research, we only consider one type of mortar configuration, a conforming mortar. A schematic of this type is depicted in Figure 11. In this case the patching process can be considered as a one-dimensional operation, with the assumption that waves are normal to the interface. As it was explained in the second chapter, a one-dimensional problem with different states on the two sides of
an interface defines a Riemann problem. Although, the solution to the Riemman problem in gas dynamics can be determined using the right and left states, but there is no closed form solution to this problem and an iterative process is often used to find the solution. Despite the availability of many exact Riemann solvers, we use the approximate Riemann solver of Roe in this work mainly because of its computational efficiency [48]. In the Roe’s method the original Riemann problem is written as

$$ q_t = A(q) q_x $$ \hspace{1cm} (4.23)

where, $A$ is the Jacobian of the matrix of the right eigenvectors of the fluxes

$$ A = \frac{\partial F}{\partial q} $$ \hspace{1cm} (4.24)
Roe’s approach replaces the Jacobian matrix by a constant Jacobian matrix

\[ \tilde{A} = \tilde{A}(q^L, q^R) \]  \hspace{1cm} (4.25)

which converts the original PDE to a linear system with constant coefficients. Now, the original Riemann problem is replaced by the approximate Riemann problem which can be solved exactly.

Using the Roe solver, the Dirichlet patching for advective fluxes yields

\[ F^{a, \text{Roe}} = \frac{1}{2} [F^a(q^L) + F^a(q^R)] - \frac{1}{2} \tilde{A} |\lambda| A^{-1} (q^R - q^L) \]  \hspace{1cm} (4.26)

where \( F^a \) is the vector of advective fluxes. For imposing inviscid boundary conditions, the physical boundary can be viewed as an interface between the external state and the computational domain. The Riemann solver is applied between the external specified flow solution and internal solution vector.

For viscous fluxes, continuity of the fluxes is established by averaging the viscous flux vector from both sides of the interface

\[ F^v = \frac{1}{2} [F^v(q^L) + F^v(q^R)] \]  \hspace{1cm} (4.27)

where \( F^v \) is the vector of viscous fluxes. The Neumann boundary conditions are imposed at the boundary points at this stage.
4.1.4 Spatial Integration

For a three-dimensional case, the integral of a generic variable $U$ can be determined as:

$$
\int_0^1 \int_0^1 \int_0^1 U(x, y, z) \, dx \, dy \, dz \cong \sum_{p=0}^{n-1} w_{p+1/2} \times \left[ \sum_{q=0}^{n-1} w_{q+1/2} \times \sum_{r=0}^{n-1} w_{r+1/2} J(X_{p+1/2}, Y_{q+1/2}, Z_{r+1/2}) \right].
$$

(4.28)

where $w_{i+1/2}$ are Legendre weights on the Legendre quadrature points and $J$ is the Jacobian matrix.

4.2 Time Integration

The differential equation obtained through spatial discretization is discretized in time with a 4th order Runge-Kutta (RK) method. This method belongs to the category of explicit time marching schemes, so that no information from previous timesteps is needed, and is also flexible and easily programmable.

The system of equations obtained after space discretization is of the following form:

$$
\frac{dq}{dt} = F(t, q(t)),
$$

(4.29)

$q(t_0) = q_0$.

(4.30)
RK methods usually are multi-staged methods and here we use a 4th order Runge-Kutta method or RK4. In RK4 the updating process is carried out as follows:

\[ q_{n+1} = q_n + \frac{1}{6} h(k_1 + 2k_2 + 2k_3 + k_4), \]  
\[ t_{n+1} = t_n + h, \]

for \( n = 0, 1, 2, 3 \). Coefficients indicated with \( k_i \) in Equation 4.31 are calculated as

\[ k_1 = F(t_n, q_n), \]
\[ k_2 = F\left(t_n + \frac{1}{2} h, q_n + \frac{1}{2} hk_1\right), \]
\[ k_3 = F\left(t_n + \frac{1}{2} h, q_n + \frac{1}{2} hk_2\right), \]
\[ k_4 = F(t_n + h, q_n + hk_3). \]

In previous equations, \( q_{n+1} \) represents the RK approximation of \( q(t_{n+1}) \), and is determined by the sum of the present value, \( y_n \), and the weighted average of four increments, each of which involves the size of the interval considered, \( h \), and an estimated slope specified by function \( F \) on the right-hand side of the differential equation.
CHAPTER 5

ENTROPY VISCOSITY METHOD FOR COMPRESSIBLE GAS DYNAMICS EQUATIONS

This chapter provides a detailed description of the implementation of entropy viscosity method in a discontinuous spectral element method (DSEM). The goal is to obtain stable and accurate numerical solution to system of Euler equations when there exist discontinuities in the flow. In the first section we discuss the regularized version of the Euler equations through adding artificial transport coefficients. The next section presents succinct mathematical formulation of the entropy based artificial viscosity. The chapter continues with describing the use of a filtering-smoothing technique as a means for achieving a smooth representation of entropy viscosity. The chapter ends with considering one and two dimensional numerical tests which clearly demonstrate the effectiveness of the method.

5.1 Regularization of Euler Equations

The original compressible Euler equations can be written in the following conservative form

\[ \frac{\partial \mathbf{q}}{\partial t} + \nabla \cdot \mathbf{F}^a (\mathbf{q}) = 0 \]  

(5.1)
where \( q = \begin{pmatrix} \rho \\ \rho u \\ e_t \end{pmatrix} \) is the vector of conserved variables and \( F^a = \begin{pmatrix} \rho u \\ \rho u \otimes u + \rho I \\ u (e_t + p) \end{pmatrix} \) is the vector of the advective fluxes. The terminology is similar to what was presented in Chapter 3, however the equations are cast into a compact form. Here, we want to formulate a regularized format of the Euler equation conforming to the technique presented in Chapter 2. For a one-dimensional conservation law, the regularized version of the hyperbolic equation was obtained through adding a dissipation term to the right hand side of the equation, which would enable us to achieve a vanishing viscosity solution of the original hyperbolic equation. Similarly, the Euler equation can be regularized by adding a vector of viscous fluxes to the right hand side as follows:

\[
\frac{\partial q}{\partial t} + \nabla \cdot F^a (q) = \nabla \cdot F^v (q) \tag{5.2}
\]

where \( F^v = \begin{pmatrix} 0 \\ \mu_h \nabla_s u \\ \mu_h \nabla_s uu + \kappa_h \nabla T \end{pmatrix} \), \( \nabla_s u \) is a symmetric tensor of rank 2 with entries \((\nabla_s u)_{i,j} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)\), \( \mu_h \) is the coefficient of dynamics viscosity and \( \kappa_h \) is the coefficient of thermal conductivity. We should note that the vector of viscous fluxes is added during the regularization process and thus all the transport coefficients are expected to be artificial. These artificial coefficients will be defined later in this chapter based on the entropy inequality for the Euler equations.
5.2 Artificial Viscosity

In the entropy viscosity method the magnitude of the artificial viscosity is proportional to the magnitude of the entropy generation. Since shocks create entropy, the magnitude of entropy generation not only indicates where the shock is located, but it also provides a measure for the artificial viscosity magnitude that smoothens discontinuities. Relatively little dissipation is added in the smooth regions to ensure an accurate computation of flow structure away from shocks. As observed in the previous section, the dissipative viscous fluxes $F_v$, are defined based on artificial transport coefficients, $\mu_h$ and $\kappa_h$, where the subscript $h$ denotes artificial coefficients. The magnitudes of the artificial diffusion coefficients are determined based on the amount of the physical entropy generation at any given point in the flow field. Formally, this is given by the amount by which the entropy transport equation deviates from a conserved equation. This quantity is called entropy residual, $D_s$:

$$D_s = \left( \frac{\partial s}{\partial t} + \nabla \cdot (us) \right)$$ (5.3)

Since, we expect the continuity equation to be conserved and to avoid loosing mass conservation because of oscillation associated with shocks and other discontinuities, we also define a residual for the continuity equation in a similar format, $D_\rho$:

$$D_\rho = \left( \frac{\partial \rho}{\partial t} + \nabla \cdot (u\rho) \right)$$ (5.4)
the total residual is then defined as the maximum of \( D_\rho \) and \( D_s \):

\[
D_h = \max \left[ \frac{\partial s_p}{\partial t} + \nabla \cdot (u_p s_p), \frac{s_p}{\rho_{h,p}} \left( \frac{\partial \rho_p}{\partial t} + \nabla \cdot (u_p \rho_p) \right) \right]
\] (5.5)

It should be remarked that the second term is multiplied by \( s/\rho \) to sustain the dimensional consistency. Now, we construct the entropy viscosity based on this residual similar to the one-dimensional formulation of artificial viscosity presented in Chapter 2. For a given solution point, \( p \) in a subdomain \( k \), we write:

\[
\mu_{h,p} |_k = \min \left( c_E h_k^2 \frac{\max_{p \in k} \rho_p}{\| s_p - \bar{s} \|_{\infty, \Omega}} R_{h,p}, c_{max} h_k \max_{p \in k} \rho_p \max_{p \in k} \left( |u| + \sqrt{\gamma RT} \right) \right)
\] (5.6)

where \( s \) is the entropy; \( h_k \) is the average grid size in each element; \( \bar{s} \) is the space-averaged entropy, and \( c_E \) and \( c_{max} \) are adjustable empirical parameters. Since, \( D_h \) is expected to oscillate at shocks we use \( R_+ = |D_h| \) instead of \( D_h \) to avoid having a negative viscosity. The first term in the parentheses is called dynamics entropy viscosity and the second term is the upper bound of entropy viscosity. The maximum viscosity is formulated using the upper bound of local wave speed \( (|u| + \sqrt{\gamma RT}) \) to ensure the stability of the numerical scheme according to the Von Neumann stability analysis presented in Chapter 2. \( \| s_p - \bar{s} \|_{\infty, \Omega} \) is the infinity norm of entropy in the whole computational domain and is used as a normalizing term to give the dynamic viscosity the dimension of viscosity.

Using non-dimensional variables and dimensionless parameters introduced in Chapter 3 we can define the non-dimensional entropy viscosity as follows:
\[ \tilde{\mu}_{h,p|k} = \frac{\mu_{h,p|k}}{\mu_f^*} = \text{Re}_f \min \left( c_E h_k^2 \max_{p \in k} \tilde{\rho}_p \tilde{R}_{h,p} c_{\text{max}} h_k \max_{p \in k} \tilde{\rho}_p \max_{p \in k} \left( |u| + \sqrt{T} \right) \right) \] (5.7)

where \( \mu_f^* \) is a reference physical viscosity, and \( \text{Re}_f \) is the Reynolds number. For Euler equations we consider \( \text{Re}_f = 1 \). The artificial thermal conductivity is proportional to the artificial viscosity by defining an artificial Prandtl number,

\[ \tilde{\kappa}_{h,p} = \frac{\gamma \text{Pr}_t}{\gamma - 1} \tilde{\mu}_{h,p} \] (5.8)

### 5.3 Entropy Viscosity for DSEM

DSEM relies upon polynomial interpolation of nodal values and presents a solution which is discontinuous across the element boundaries. The original EV method treats these small jumps as discontinuities and may become highly irregular and non-smooth near shocks. While setting the constants \( c_E \gg 1 \) and \( c_{\text{max}} \gg 1 \) can alleviate this problem and help stabilize the incipient numerical oscillations, it might adversely affect the method’s ability to preserve the correct wave amplitude. A tailored version of the EV method for DSEM, capable of providing smooth distribution of entropy viscosity allows for the use of much smaller \( \mu_h \), which provides higher accuracy.

The implementation of the entropy viscosity method in DSEM requires attention to a number of components of the algorithm including entropy viscosity residual construction, values of the model parameters, and smoothing the viscosity. These will be discussed below.
5.3.1 Entropy Viscosity Residual Construction

The construction of entropy viscosity residual requires the evaluation of both time and spatial derivatives of density, entropy and entropy fluxes $f^1 = us$, $f^2 = u\rho$. The entropy and entropy fluxes are first calculated at the Gauss-Gauss points and are then interpolated to the Lobatto points. An approximate Riemann solver based on the Roe-Pike method [48] is then used at the interfaces to determine the fluxes. Despite the Riemann solver used for advective fluxes, here we use the Riemann solver to determine the average states or Riemman solutions instead of the fluxes. Assuming two given states at the sides of an interface as

$$
q^L = \begin{pmatrix}
\rho^L \\
\rho^L u^L \\
\rho^L v^L \\
\rho^L w^L \\
e^L_I
\end{pmatrix}, 
q^R = \begin{pmatrix}
\rho^R \\
\rho^R u^R \\
\rho^R v^R \\
\rho^R w^R \\
e^R_I
\end{pmatrix}
$$

the average vector $\bar{q}$ is given by
\[
\begin{aligned}
\tilde{\rho} &= \sqrt{\rho^L \rho^R}, \\
\tilde{u} &= \frac{\sqrt{\rho^L u^L} + \sqrt{\rho^R u^R}}{\sqrt{\rho^L} + \sqrt{\rho^R}}, \\
\tilde{v} &= \frac{\sqrt{\rho^L v^L} + \sqrt{\rho^R v^R}}{\sqrt{\rho^L} + \sqrt{\rho^R}}, \\
\tilde{w} &= \frac{\sqrt{\rho^L w^L} + \sqrt{\rho^R w^R}}{\sqrt{\rho^L} + \sqrt{\rho^R}}, \\
\tilde{H} &= \frac{\sqrt{\rho^L H^L} + \sqrt{\rho^R H^R}}{\sqrt{\rho^L} + \sqrt{\rho^R}}, \\
\tilde{c} &= \left( \frac{\gamma - 1}{2} \right) \left( \tilde{H} - 1/2 \tilde{V}^2 \right). 
\end{aligned}
\]  

(5.9)

where \( \tilde{V}^2 = \tilde{u}^2 + \tilde{v}^2 + \tilde{w}^2 \), \( \tilde{H} \) and \( \tilde{c} \) are the average state enthalpy and speed of sound, respectively.

The entropy fluxes are then calculated using their functional relations with the average solution variables.

Although the entropy generation equation is not integrated in time like the conservation laws, but the calculation of the entropy does require the approximation of a time derivative. This renders the use of the fourth-order Runge-Kutta scheme, that is used for time integration of the conservation laws, impractical. Instead, the time derivative is evaluated with a second-order backward difference method as follows:

\[
\frac{\partial \phi^n}{\partial t} = \frac{1}{2\Delta t} \left( 3\phi^n - 4\phi^n - 1 + \phi^{n-2} \right) + O[(\Delta t)^2]
\]

(5.10)

where \( \phi = s \) or \( \rho \), and \( \Delta t \) is the time step size. The backward differencing scheme requires the storage of the entropy and density at \( t^{n-1} \) and \( t^{n-2} \). With the entropy viscosity residual known,
the artificial transport coefficients $\mu_h$ and $\kappa_h$ can be determined at $t^n$ and the conservation laws can be integrated in time.

5.3.2 Model Parameters

Parameters $c_E$ and $c_{max}$ are problem dependent and for any given problem, a coarse mesh computation determines these parameters. First we set $c_E = \infty$ and adjust $c_{max}$ until a stable and smooth solution is achieved. Having set the $c_{max}$ and $c_E$ is decreased until the simulation is on the verge of losing stability or smoothness. This procedure, guarantees a smooth and essentially oscillation free solution. Since this approach yields a unique set of $c_{max}$, $c_E$ for any given mesh, the accuracy of the solution will be mainly determined by the number of elements and the polynomial order. The magnitudes of $c_E$ and $c_{max}$ are not independent of the selected polynomial order and this procedure should be repeated for any chosen $\mathcal{P}$.

5.3.3 Smoothing the Viscosity

A smooth variation in artificial viscosity benefits the dynamics of the simulation and improves robustness and accuracy. Specifically in DG, jumps in viscosity from one element to the next along a discontinuity, introduce errors to the solution in both normal and tangential directions to the shock front. These errors create variations in the flow field which can convect downstream and pollute the solution accuracy [44]. Several research efforts [44, 45, 55] have proposed methods to achieve a smooth representation of the artificial viscosity mainly by coupling a reaction-diffusion type PDE to the system of equations. Despite its success in many space discretization and time integration schemes, this approach results in a stiff system of ODEs which is too restrictive on an explicit time step. Recently, Premasuthan et al. [56] imple-
mented an artificial viscosity method in spectral difference method for high-order computation of compressible flows and used a dilatation-based switch and filter for smoothing that led to good results on unstructured grids. In this research, we also propose a new filtering-smoothing procedure to achieve a smooth and localized artificial viscosity for high-order computation of compressible flows.

5.3.3.1 Element Level Filtering

Filtering is used as a part of our approach to capture shocks and stabilize the solution while preserving high-order resolution. We employ a spectral low pass explicit filter to remove oscillations from the solution values and their derivatives at each time step. In this work, an element based interpolation-projection filtering approach is utilized following Blackburn and Schmidt [57]. Numerical experiments show that higher-order polynomial orders can leave some oscillations in the flow field, especially near flow discontinuities, and subsequently exhibit an adverse effect on solution derivatives and potentially entropy viscosity distribution. These high-frequency oscillations can be filtered without altering the main features of flow with the filtering procedure explained below. The specific spectral filter dampens high-frequency oscillations, yielding a smooth representation of the solution while ensuring inter-element continuity.

In the filtering procedure, the filtered polynomial function of degree $N$ is obtained by projecting it to and from a lower order approximation of degree $M$ defined on a subset of the original nodal values. First, the polynomial $P_N$ of degree, $N$, is interpolated to a polynomial $P_M$ of lower degree $M$,
\[ Q'(x_i) = \sum_{j=0}^{N} Q(\bar{x}_j) l_j(x_i) \quad (5.11) \]

where \( ' \) shows the interpolated function, and \( x_i \) and \( \bar{x}_j \) are the nodes corresponding to \( P_M \) and \( P_N \), respectively. Here, \( l_j \in P_N \) is the Lagrange interpolating polynomial. The above operation can be presented in terms of matrix-vector products

\[ Q'_i = I^\text{int}_{ij} Q_j, \quad (5.12) \]

where \( I^\text{int}_{ij} \) is the interpolation matrix,

\[ I^\text{int}_{ij} = \prod_{k=0,k\neq j}^{N} \frac{x_i - \bar{x}_k}{\bar{x}_j - \bar{x}_k}, \quad i = 0, ..., M, \quad j = 0, ..., N. \quad (5.13) \]

In the second step, the function \( Q'(x) \) is projected back to the polynomial space \( N \) giving the filtered variables \( Q^\text{filt} \),

\[ Q^\text{filt}(\bar{x}_e) = \sum_{f=0}^{N} Q'(x_f) l_f(\bar{x}_e) \quad (5.14) \]

the above operation can be cast in matrix-vector product form as,

\[ Q^\text{filt}_e = I^\text{proj}_{ef} Q'_f \quad (5.15) \]
where $P_{ef}^{proj}$ is the projection matrix,

\[ P_{ef}^{proj} = \prod_{k=0, k \neq f}^{M} \frac{\bar{x}_e - x_k}{x_f - x_k}, \quad e = 0, \ldots, N, \quad f = 0, \ldots, M. \tag{5.16} \]

Figure 12 shows a schematic of the filtering operation showing the transformation of a rather noisy original data to a smoother distribution after filtering.

In the staggered grid method, this interpolation-projection operation could be applied to both of the nodal sets (Gauss-Gauss and Gauss-Lobatto nodes). We apply the filter on the Gauss-Lobatto basis since it preserves the edge/boundary of the original function and ensures $C_0$ continuity. Finally, we introduce the filter strength parameter, $\alpha$, to control the filtering strength,

\[ Q(\bar{x}) = (1 - \alpha) Q^{filt}(\bar{x}) + \alpha Q(\bar{x}) \tag{5.17} \]

5.3.3.2 Smoothing Operator

A two dimensional smoothing operator, which was also used by Guermond et al. [46], is employed to further smooth the entropy viscosity once the viscosity is projected to the Lobatto points. This operator is defined as

\[ S[\phi(\xi, \eta)] = \frac{1}{8} \left[ 4\phi(\xi, \eta) + \sum_{i=1}^{4} \phi_i(\xi_i, \eta_i) \right] \tag{5.18} \]
where $\phi_i$ represent the values of function $\phi$ at the neighboring points $(\xi_i, \eta_i)$ of the point of interest. Note that the neighboring points can be on a different element. In case the node is on an interface or at the corner of the Gauss grid, the magnitude of $\phi$ is not unique because of the discontinuous nature of the method. In this event, an averaged magnitude of $\phi$ is obtained by considering all the participating neighbors in the above smoothing operator.

### 5.3.3.3 Smoothing-Filtering Procedure

In this work a combination of smoothing and filtering is employed to achieve a smooth artificial viscosity. Different strategies have been tested and what follows has proven to produce the best results. At any time step we implement the following procedure to calculate the entropy viscosity:

1. Explicitly filter the solution values, $q_k$, at Gauss-Gauss points over each element. Filtered values are denoted as $\bar{q}_k$. 

Figure 12: Illustration of filtering using interpolation-projection
2. Calculate entropy values using $\overline{q}_k$ at the Gauss-Gauss points and interpolate to Lobatto points.

3. Construct the entropy fluxes at the Lobatto grid, denoted as $f_K$.

4. Evaluate the entropy flux derivative at the Gauss-Gauss points using $f_K^e$, and then calculate the entropy viscosity $\mu_{gg}$ at these points.

5. Smoothen $\mu_{gg}$ using the smoothing operator, $S$, over all Lobatto points.

6. Obtain $\mu_{gl}$ and $\mu_{lg}$, by interpolating $\mu_{gg}$ to the Gauss-Lobatto points and the Lobatto-Gauss points to, respectively.

5.4 Numerical Experiments

5.4.1 One-Dimensional Test Problems

In this section we focus on the simulation of the shock tube problem where we consider two different test cases, namely, Sod and Lax problems. A schematic of a shock tube is shown in Figure 13 where we see two distinct sections in the tube, high pressure and low pressure, which are initially separated by a diaphragm. Once the diaphragm is ruptured the difference in pressure and density between the high pressure driver gas and the low pressure driven gas will create an expansion wave, a shock wave and a contact surface. For more detail on shock tube operation and physics we refer to [58].

In this section we are going to perform numerical simulation of the shock tube problem and compare the obtained results against the available exact solution to this problem. As it was mentioned in the first part of this chapter, artificial dissipation should be added to the solution
in the vicinity of the shock in order to capture the shock. As presented in the formulation of the entropy viscosity method, the magnitude of the artificial viscosity is determined based on the entropy residual which is allegedly large at shocks and negligible in smooth areas. Before we begin to present the detail of the one-dimensional simulation, it would be appropriate to perform a quantitative study on the behavior of entropy residual in a simple problem.
We consider a transition in fluid properties under two different scenarios. First, we let the transition happen gradually in a way that there is no sudden change in fluid properties. Figure 14 shows the variation of density and velocity in this case. Following the conclusions of previous section, we expect the entropy residual to be negligible in this case. Figure 15 shows the temporal and spatial derivatives of entropy for this case and as we expected the net of entropy generation is almost zero where the change in fluid properties is smooth. On the contrary, if the change is sudden similar to what we have in shock waves, we expect to observe a jump in entropy. This expectation is supported by our numerical experiment. If we consider a similar test case but with a rather sharp drop in density and velocity as depicted in Figure 14, the net entropy generation is nonzero (See Figure 15).

Figure 14: Variation of (a) density and (b) velocity in entropy residual study under two transition scenarios; sharp and smooth
Sod Problem

In the first test case, we consider the Sod shock tube problem. We solve the Euler equations subject to the following initial data [48]:

\[(\rho, u, p) = \begin{cases} 
(1.0, 0.75, 1.0) & \text{if } x < 0.5; \\
(0.125, 0, 0.1) & \text{if } x \geq 0.5. 
\end{cases}\]

This specific initial condition gives rise to a contact wave moving to the right, and a strong right traveling shock wave. Simulations are carried out on a mesh of 100 $P^3$ (i.e. polynomial order 3) elements and the results are analyzed at time $t = 0.2$. Model parameters $c_E = 1.0$ and $c_{\text{max}} = 0.5$ have been used for this problem. A comparison between the exact solution and the
DSEM-EV solution for the density, pressure, velocity and temperature is shown in Figure 16. A good agreement between the simulation results and the exact solution is observed. In particular, the positions of both the contact discontinuity and the right propagating shock are accurately captured. DSEM-EV gives nearly identical solutions as compared to the analytical solutions. The contact surface is also sharply resolved due to the method’s ability to distinguish between a shock wave and a contact discontinuity. In this configuration, the jumps in pressure and temperature are challenging to capture at the shock wave location. As it is clearly seen from the results, DSEM-EV is able to capture the shock within only a few solution points.

**Performance of the Smoothing-Filtering Operator**

In Figure 17 we assess the relative smoothness of the viscosity obtained using DSEM-EV method as opposed to the original entropy viscosity method. The Sod shock tube problem is used for this study. In Figure 17(a) it is observed that the DSEM-EV provides a smooth distribution of $\mu_h$ compared to that from the original approach while providing smaller dissipation at the contact discontinuity.

Alternatively, in Figure 17(b) we plot the density distribution obtained using DSEM-EV in comparison to that from the original approach. Both plots demonstrate that DSEM-EV provides smoother yet more localized dissipation where it is needed (at the shock wave) and minimizes the added dissipation at the contact surface resulting in a sharper density profile.

**Mesh Refinement Study**

Figure 18(a) shows the effect of mesh refinement on the density distribution. Figure 18(b) displays the effect of p-refinement on the results. As it is expected, increasing mesh resolution
either by increasing the polynomial order or the number of elements, improves the solution accuracy and shock resolution. The number of solution points in three different cases used for h and p-refinement studies is the same and lines with the same color have the same number of solution points. It can be seen that, between cases with the same number of solution points, a more accurate solution can always be achieved when a higher polynomial order is used. This is also desired in terms of the computational cost as using high-order elements reduces the computational time.
Figure 17: A comparison between results produced by the DSEM-EV method and the original entropy viscosity approach for the Sod shock tube problem at $t = 0.2$. (a) Entropy viscosity and (b) density.

Lax Problem

In the second test case, we consider the Lax shock tube problem with the initial data

$$(\rho, u, p) = \begin{cases} 
(0.445, 0.698, 3.528) & \text{if } x < 1; \\
(0.5, 0, 0.571) & \text{if } x \geq 1.
\end{cases}$$
Figure 18: Effect of grid refinement on density variation for the Sod problem (a) h-refinement with $P3$ elements (b) p-refinement using 100 elements.

Figure 19: Comparison of results for the Lax problem obtained using DSEM-EV with the exact solution at $t = 1.8$. 
This case is computed on a mesh with 100 $P^5$ elements and the results are analyzed at time $t = 0.2$. The initial values specified above give rise to strong contact and shock discontinuities. The comparison between the exact solution and DSEM-EV result is shown in Figure 19.

Effect of Model Parameter $c_E$

In this example, we take different values of the viscosity coefficient $c_E$ in order to demonstrate the effect of $c_E$ on the results. We begin with $c_E = 0.1$ which is the smallest value of this parameter producing stable results. As shown in Figure 20, the computed density is very oscillatory near the contact and shock discontinuities. From the results, shown in Figure 20 for increasing values of $c_E = 0.25, 0.5, 1, 2$ and 4, we conclude that $c_E = 1$ is optimal. Following the procedure explained in Sec. 3.2.2, we chose $c_{\text{max}} = 0.5$, the same values of $c_E$ and $c_{\text{max}}$ were used for the results shown in Figure 19.
Figure 20: Density computed by DSEM-EV with different values of $c_E$ for the Lax problem.

Solid line represents the exact solution.
5.4.2 Two-dimensional Test Problems

5.4.2.1 Explosion Problem

As our first 2D test case, we consider the explosion problem for an ideal gas with $\gamma = 1.4$. The geometry and initial conditions are such that cylindrical symmetry can be enforced. The 2D Euler equations are solved on a $2.0 \times 2.0$ square domain in the $x$-$y$ plane. The initial condition consists of the region inside of a circle with radius $R = 0.4$ centered at $(1, 1)$ and the region outside of the circle. The flow variables are constant in each of these regions and are separated by a circular discontinuity at time $t = 0$. The two constant states are chosen as

\[
\begin{align*}
    u_{\text{in}} &= 0 ; \quad u_{\text{out}} = 0 \\
    v_{\text{in}} &= 0 ; \quad v_{\text{out}} = 0 \\
    \rho_{\text{in}} &= 1.0 ; \quad \rho_{\text{out}} = 0.125 \\
    p_{\text{in}} &= 1.0 ; \quad p_{\text{out}} = 0.100
\end{align*}
\]

where subscripts $\text{in}$ and $\text{out}$ denote values inside and outside the circle, respectively. We solve the full 2D Euler equations using our DSEM-EV code. The simulations are carried out on a mesh consisting of 2500 $P^7$ elements and the results are analyzed at time $t = 0.25$. Wave transmissive boundary condition is assigned to all boundaries. It was necessary to smoothen the initial discontinuity over a few grid points in order to stabilize the simulation. Model parameters $c_E = 0.4$ and $c_{\text{max}} = 0.2$ have been used for this problem.
Figure 21: Contours of (a) density (b) pressure (c) velocity (d) temperature for the explosion problem.

Figure 21 shows that the radial discontinuities are resolved sharply, while the symmetry of the flow is captured on the 2D Cartesian grid. Figure 22 shows a comparison between the 1D exact solution [48] and the 2D DSEM-EV solution along the radial line along with the x-axis for the density, pressure, horizontal velocity and temperature. Comparisons along any radial line give identical results. The shock wave is resolved within one element. Although the contact discontinuity is challenging to resolve, Figure 22 shows that this discontinuity is also sharply
resolved with the modified entropy viscosity method. Figure 23 displays the time evolution of the entropy viscosity in this problem. It is observed that the entropy viscosity is localized to the area of contact discontinuity and shock wave, and is almost negligible in other areas. Despite the use of a high-order polynomial in this case the distribution of viscosity is smooth throughout the domain throughout the simulation.

![Graphs of radial variations](image)

Figure 22: Comparisons of radial variations of (a) density (b) pressure (c) velocity (d) temperature obtained using DSEM-EV with the exact solution.
Figure 23: Spatial variation of entropy viscosity at different times for the explosion problem.
5.4.2.2 Flow Over a Forward-Facing Step

To further test the performance of the 2D DSEM-EV Euler code, a Mach 3 flow over a forward-facing step is considered here. The problem was originally introduced by Emery [60] to compare several schemes in classical fluid dynamics. Figure 24 shows the geometry and boundary conditions used in the problem. Initially the tunnel is filled with a gas, with adiabatic coefficient $\gamma = 1.4$, uniform density $\rho = 1.4$, pressure $p = 1.4$, and velocity $\mathbf{v} = (3, 0)$.

Figure 24: Geometry and boundary conditions for the Mach 3 flow over a forward-facing step in a wind tunnel.

A constant inflow boundary condition is applied at the left end of the computational domain and a transmissive outflow boundary condition is implemented at the right end. Slip boundary condition is applied to upper and lower walls and a adiabatic wall boundary condition is applied
to the vertical step wall. The flow configuration has a singularity which is the corner of the step. This singular point is the center of a rarefaction fan. The singularity can potentially lead to an erroneous entropy layer attached to the bottom wall as well as some unpredictable density oscillations near the Mach stem. In this study and unlike in some previous work \[60,61\], the scheme is not modified near the corner, neither is the mesh refined. This will allow us to evaluate the influence of large elements with high-order approximation in the entropy layer.

Figure 24 depicts the density contours in 0.5 time intervals obtained using a mesh of 14,175 $P^3$ elements. It is noted that the computations are stable without corner treatment. Figure 26 displays the comparison of density contours at $t = 3.0$ against the results obtained using a second-order quiet direct simulation (QDS) by Smith et al. \[5\] which is one of the most accurate results in the literature and shows good consistency with other references.
Figure 25: Contours of density obtained using 14,175 $P3$ elements for Mach 3 flow over a forward-facing step.
Figure 26: Contours of density obtained using 14,175 $P^3$ elements for Mach 3 flow over a forward-facing step (continued).
Figure 27: Plots of entropy viscosity at time intervals of 0.5 for a Mach 3 flow over a forward-facing step.
Figure 28: Plots of entropy viscosity at time intervals of 0.5 for a Mach 3 flow over a forward-facing step (continued).

Our results show that DSEM-EV effectively captures almost all features of the flow field and that the results compare very closely with other published results. One feature which is not
Figure 29: Contours of density at $t = 4.0$ for Mach 3 flow over a forward-facing step in a wind tunnel obtained using DSEM-EV (a) and from the results of Smith et al. [5] (b).

captured accurately is shock system detachment from the bottom wall. The solution accuracy is also altered to an extent near the bottom wall. Although, this issue can be resolved by implementing special boundary treatment in this area [62], but this modification can not be physically justified. In Figure 29 (a) 2D plot of the entropy viscosity is shown at the final time, where the entropy viscosity is clearly present only in the shocked areas and the singular corner point.
5.4.2.3 Two-dimensional Rayleigh - Taylor Instability

In this section we try to use our shock capturing method to simulate a fluid discontinuity problem between two different gases where small perturbations at the interface can grow into nonlinear structures having the form of spikes. We use the EV method to stabilize these spikes through adding dissipation at the interface of the two fluids. We model the Rayleigh-Taylor instability by means of the two-dimensional Euler equations evolving an initial perturbed interface separating two states of a fluid, light and heavy. This is a buoyancy driven flow, and we shall introduce a source term in the original Euler equations. The relevant source term vector has a form of $\mathbf{S} = (0, 0, \rho, 0, \rho v, 0)$. The instability occurs when heavier and lighter fluids are drawn into each other by the gravity. When evolving in time the unstable regime at the interface is excited through the acceleration of gravity and bubbles of the lighter fluid rise into the heavier fluid and spikes of heavier fluid fall into the lighter fluid. Since the simulation is done for an inviscid flow, the material interface between the two fluids should continue to break down into smaller and smaller structure. Numerical dissipation can prevent this trend and on the contrary adding too much artificial dissipation can create crude interface resolution and pretty much does not allow the scheme to capture smaller flow structures [63].
Figure 30: Plot of density at 0.4 time intervals for the inviscid Rayleigh-Taylor instability problem.
The flow variables are initialized as:

\[
(\rho, u, v, p) = \begin{cases} 
(1.0, 0.0, -0.025c \cos(8\pi x), y + 1.5) & \text{if } 0.5 \leq y \leq 1.0; \\
(2.05, 0.0, -0.025c \cos(8\pi x), 2y + 1.0) & \text{if } 0.0 \leq y < 0.5.
\end{cases}
\]

where \(c\) is the local sound speed. Reflective boundary conditions are used for the left and right walls and following boundary conditions and are set for the upper and lower boundaries:

\[
(\rho, u, v, p) = \begin{cases} 
(1.0, 0.0, 0.0, 2.5) & \text{if } y = 1.0; \\
(2.05, 0.0, 0.0, 1.0) & \text{if } y = 0.0.
\end{cases}
\]

The computational domain has the dimensions of \([0, 0.25] \times [0, 1]\) with a total of 900 \(P3\) elements. Figure 30 shows the density contours evolution in time and it is clearly observed that the EV method is able to capture very fine structures even on a relatively coarse grid. Figure 31 compares the density contour obtained by EV method to density contours obtained using WENO 63 and a shock fitting method 63. It is clearly observed that the results of EV scheme show more small-scale structures than those by the WENO and shock fitting scheme for the same grid resolution. This confirms that the numerical dissipation of EV schemes are lower than other shock capturing schemes.
Figure 31: Density contours in the inviscid Rayleigh-Taylor instability problem as predicted by WENO5, MP5, and MP7 schemes in comparison with EV. In all figures, 15 contour lines ranging from 0.95227 to 2.14589 are considered.
CHAPTER 6

EXTENSION OF ENTROPY VISCOSITY METHOD TO NAVIER-STOKES EQUATIONS

In the previous chapter, we demonstrated the successful implementation of entropy viscosity method in our spectral element method code, as a means to capture shock waves and other discontinuities gas dynamics problems through adding localized artificial viscosity. In this chapter, we present a new formulation for EV method which enables us to extend the use of EV method to viscous flows. The potential of the method and its improved accuracy and numerical stability is illustrated by several test cases.

6.1 Shock and Turbulence Interaction

As it was mentioned in the first Chapter, many applications in science and engineering involve the interaction of shock waves and turbulent flows. A prime example is the flow around aerodynamic bodies and through propulsion system of high-speed flight vehicles.

With an increasing body of direct numerical simulation (DNS) or large-eddy simulation (LES) work, it has become evident that traditional low-order numerical methods, often used for RANS computations, do not yield sufficiently accurate DNS and LES results. This has prompted a surge in the development of high-order methods offering for turbulence simulation over the last decade. Discontinuous Spectral Element Method (DSEM) is a notable member of this high-order family of methods. The low-dispersion and low-diffusion error nature of DSEM
makes it an excellent candidate for turbulence simulation. However, in compressible turbulence simulation using an artificial viscosity based shock capturing method for DNS or LES turbulence simulation can impose conflicting demands on the numerical algorithm. In one hand, spurious oscillations form near shocks and and other flow discontinuities which can drastically degrade the quality of the solution and need to be dampened by means of artificial viscosity. On the other hand, capturing broadband spatial and temporal variations in a turbulent flow requires adding minimal dissipation and dispersion, a condition which can be easily violated if the shock capturing scheme adds dissipation to natural oscillations associated with turbulence. Almost all artificial viscosity based shock capturing methods are capable of detecting shocks, and resolving them in the absence of strong physical oscillation although the level of accuracy may vary from one method to another. However, when dealing with turbulence, the shock capturing switch might be triggered by strong oscillations associated with turbulence leading to over-damping the turbulence and yielding poor turbulence resolution and statistics. Therefore, shock capturing scheme must be able to distinguish between shock waves and strong turbulence oscillations and selectively add dissipation to shock waves so that they can be captured, while preserving high wave number oscillations in the turbulent field.

The main objective of this chapter is to evaluate the performance of the entropy viscosity method on compressible turbulent flows with shocks. We develop and validate a modified version of our shock capturing scheme, which is adequate for capturing shocks in supersonic flows and resolving interactions between shocks and turbulence.
6.2 Modified Entropy Viscosity Method for Viscous Flows

Although the implementation of the original EV method enables stabilizing compressible turbulent flows and resolving shock waves and other discontinuities but it also incurs some penalties on the turbulence statistics. This is mainly because of the excessive dissipation on dilatational modes and also pressure, density and temperature fluctuations, which in turn leads to an undesirable decay in turbulent kinetic energy and spectra. Here, we propose a new formulation based on the original idea of entropy viscosity method for turbulent flows. Emphasis is placed on the improvement of the entropy residual by employing a modified version of residual based on the entropy transport equation. In addition, we utilize a switching function (shock sensor) to enable the method to differentiate between shocks and turbulence oscillations. This allows us to reduce the dissipation in the smooth areas and impart more selectivity to artificial dissipation. Theses modifications are discussed in the following subsections.

6.2.1 Modified Entropy Residual

In the formulation of entropy viscosity method for gas dynamics governed by Euler equations, we defined the entropy residual based on the entropy inequality for Euler system of equations:

\[ D_s = \left( \frac{\partial s}{\partial t} + \nabla \cdot (us) \right) \geq 0 \]  \hspace{1cm} (6.1)

which gives a measure for the amount by which the system deviates from an isentropic process, which in the EV method, is used as a means for locating shock waves in the flow. When dealing with viscous flows, the above equation is not valid and one should write the entropy
residual based on the full form of entropy transport equation, presented in Chapter 3. The non-dimensional entropy residual based on entropy transport equation for Navier-Stokes system of equations reads:

$$\frac{D\rho s}{Dt} - \left[ \frac{1}{Re_f T} \Phi + \frac{1}{Pr_f Re_f (\gamma - 1)M_f^2 T} \Gamma + \frac{1}{Pr_f Re_f (\gamma - 1)M_f^2} \Lambda \right] > 0 \quad (6.2)$$

where,

$$\Phi = 2 \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 + \left( \frac{\partial w}{\partial z} \right)^2 \right] + \left[ \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)^2 \right] - \frac{2}{3} \left[ \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right] \right]$$

$$\Gamma = \left[ \left( \frac{\partial T}{\partial x} \right)^2 + \left( \frac{\partial T}{\partial y} \right)^2 + \left( \frac{\partial T}{\partial z} \right)^2 \right] \right]$$

$$\Lambda = \left[ \frac{\partial}{\partial x} \left( \frac{1}{T} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{1}{T} \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( \frac{1}{T} \frac{\partial T}{\partial z} \right) \right].$$

In the above equation, $\Phi$ and $\Gamma$ are the entropy generation terms due to viscous dissipation and heat conduction within the flow, respectively. These terms are always positive and can be of importance in the areas where large velocity and temperature gradients exist. These terms are positive where larger turbulence oscillations appear in the flow and considering the new form of the residual inhibit any unwanted dissipation in the smooth areas due to these terms.

It should be pointed out that the entropy transport equation remains a conservation equation provided the flow is not affected by shock waves. The entropy transport equation holds a
balance between entropy material derivative and entropy transport terms due to heat transfer and viscous dissipation. We illustrate this fact by considering a simple example where the flow experiences large velocity and temperature gradients but there is not shocks. We consider a $[0, 5]^3$ box with a sharp temperature and velocity distribution in three dimensions imposed as initial conditions. Figure 32 shows a slice of velocity and temperature distribution through $z = 2.5$ plane. In this case we seek a balance in the form of

$$\frac{D\rho s}{Dt} = \left[ \frac{1}{Re_f} \frac{\Phi}{T} + \frac{1}{Pr_f Re_f (\gamma - 1) M_f^2 \Gamma} + \frac{1}{Pr_f Re_f (\gamma - 1) M_f^2 \Lambda} \right]. \quad (6.3)$$

Figure 33 plots the spatial variation of the terms on the LHS of the above equation in comparison with the spatial variation of the terms on the RHS through the $z = 2.5$ plane after a few time steps. As it can be seen from this comparison and also from the line-plot depicted in Figure 34, the entropy transport equation holds a balance for this case despite the existence of large gradients. This is a strong conclusion as it behaves as a powerful means to distinguish between shocks and strong oscillation in the flow.

6.2.2 Shock Sensor

As mentioned before, a practical modification in the design of a shock capturing method for viscous and specially turbulent flows would involve incorporating a shock switch which turns on only in shocked regions thus removing unwanted dissipation in other regions like expansion waves or turbulence. The general form of the artificial viscosity can be written as

$$\mu_h = C_{\mu} \rho D_{\mu} h^2 \quad (6.4)$$
where $C_\mu, D_\mu$ and $h$ are an user defined constant, a residual and grid spacing, respectively. One can incorporate a shock switch, $F_{sw}$, in the above formula and introduce a new form for the artificial viscosity as:

$$\mu_h = F_{sw}C_\mu \rho D_\mu h^2$$  \hspace{1cm} (6.5)

This model enables us to localize the artificial bulk viscosity only near shock waves. It is known that shocks are regions of strong compressive waves creating high negative dilatation (strong compression waves), and on the contrary strong turbulence can often be characterized by strong
vortisity. This notion, forms the basis of the shock sensor used in this research, which was first proposed by Ducros [64] in the form:

$$\mathcal{F}_{\text{Ducros}} = \frac{(\nabla \cdot \mathbf{u})^2}{(\nabla \cdot \mathbf{u})^2 + |\nabla \times \mathbf{u}|^2 + \epsilon}$$

(6.6)

where $\epsilon$ is a very small positive number to prevent a division by zero in the areas where velocity divergence and vortisity are both zero. This function varies between 0 for weakly compressible regions to about 1 in shock regions. The proposed shock sensor in this research is the combination of a negative dilatation sensor $H(-\nabla \cdot \mathbf{u})$ and the Ducros-type sensor

$$\mathcal{F}_{sw} = H(-\nabla \cdot \mathbf{u}) \frac{(\nabla \cdot \mathbf{u})^2}{(\nabla \cdot \mathbf{u})^2 + |\nabla \times \mathbf{u}|^2 + \epsilon}$$

(6.7)
Figure 34: Density variation in the Shu-Osher problem at $t = 1.8$ obtained with DSEM-EV using 200 $P3$ elements compared with results using the WENO scheme

where $H$ is the Heaviside function. The negative dilatation switching removes the unnecessary viscosity from expansion regions and the Ducros-type sensor reduces the bulk viscosity at weakly compressible regions without shocks induced by the motions of turbulent eddies.

### 6.2.3 Implementation Details

In the previous chapter we presented the EV formulation for Euler equations and presented the regularized form of the Euler system introducing a vector of viscous fluxes based on artificial transport coefficient $\mu_h$ and $\kappa_h$. But despite the Euler equations and according to equations presented in Chapter 3, the Navier-Stokes system of equations has a vector of viscous fluxes based on physical transport coefficients $\mu_p$ and $\kappa_p$ and the artificial transport coefficients should naturally be added to their physical counter parts providing additional dissipation in the areas of
flow discontinuity. Therefore, in our numerical scheme the viscous fluxes should be constructed based on the augmented transport coefficients

\[
\mu = \mu_p + \mu_h \\
\kappa = \kappa_p + \kappa_h,
\]

(6.8)

Recalling the non-dimensional form of the entropy viscosity from previous chapter and considering the proposed modifications in this chapter we can write the artificial viscosity for viscous flows as

\[
\mu_{h,p}|_k = F_{sw} \left[ \text{Re}_f \min \left( c_E \hat{\kappa} \frac{\max_{p \in k} \rho_p}{R_{h,p}} c_{h,p} \max_{p \in k} \max_{p \in k} \left( |u| + \sqrt{T_M} \right) \right) \right]
\]

(6.9)

where

\[
R = \left| \frac{D\rho_s}{Dt} - \left[ \frac{1}{\text{Re}_f T} \Phi + \frac{1}{Pr_f \text{Re}_f (\gamma - 1) M_f^2} \Gamma + \frac{1}{Pr_f \text{Re}_f (\gamma - 1) M_f^2} \Lambda \right] \right|
\]

(6.10)

and \( F_{sw} \) is calculated using Equation 6.7.

6.3 Numerical Tests

6.3.1 Shu-Osher Problem

we consider the Shu-Osher problem that involves the interaction of a Mach 3 shock and a sinusoidal density wave. This benchmark problem can be considered as a one-dimensional model to study shock-turbulence interaction. The initial conditions for this problem are described as
\[ (\rho, u, p) = \begin{cases} 
(3.857143, 2.6269369, 10.333333) & \text{if } x < 1; \\
(-1 + 0.2 \sin(5x), 0, 1) & \text{if } x \geq 1.
\end{cases} \]

The computational domain is \([0, 10]\), discretized with a uniform mesh of 200 \( P3 \) elements equivalent to 800 grid points. Model parameters \( c_E = 1 \) and \( c_{\text{max}} = 0.5 \) have been used for this problem. We analyze the solution at \( t = 1.8 \). At this time, downstream the \( Ma = 3 \) shock, there exist both shocklets and entropy waves. In Fig. [Figure 35] the density variation is compared against the solution obtained with a fifth-order WENO scheme on 4000 points [33]. Despite the smaller number of grid points used in our simulation, the density waves are preserved well without noticeable spurious oscillations around the shocklets.

6.3.2 Decaying Isotropic Turbulence

To test the performance of the developed method for compressible turbulence simulation we consider the problem of decaying isotropic turbulence inside a periodic box. This 3D test case presents a simple and efficient way for the evaluation of the dissipation characteristics of the shock capturing models. At a sufficiently high turbulent Mach number, weak shock waves (eddy shocklets) develop spontaneously in the flowfield and since the location of these shocklets are now known apriori it can pose a challenge to the shock capturing method as it needs to dynamically locate and resolve these shock surfaces. Initially, we discuss the general framework in which we set up the problem including the initial condition details and turbulence modeling using explicit filtering. Subsequently, a test simulation is performed and results are analyzed for a low \( rms \) Mach number case to test the problem setup and validate the results against the
available results in literature. The rest of the compressible isotropic simulations are used to assess the performance of the shock capturing method.

6.3.2.1 Problem Setup

Computation of the decaying isotropic turbulence is performed within a periodic box of size $2\pi$. To perform the simulations, initial conditions for the dependent variables must be specified which should generate an isotropic and periodic field for the velocity and thermodynamics variables. In isotropic turbulence, initial conditions are parametrized by an $rms$ fluctuation level and the shape of the three dimensional correlation spectrum. Here we follow the procedure outlined by Blaisdel [65] to setup the initial field. For simulations considered in this chapter, we
consider the thermodynamic variables to be divergence free in the beginning of simulation and thus the mean values only need to be specified. On the contrary, the velocity field has rms in all three directions which are determined from a velocity correlation spectrum. The velocity field can be decomposed into two parts,

\[ u = u^s + u^d \]  

(6.11)

where

\[ \nabla \cdot u^s = 0 \quad , \quad \nabla \times u^d = 0 \]  

(6.12)

\( u^s \) is the solenoidal velocity component and \( u^d \) is the delaitational velocity component and a relative rms level of these two velocities are usually given. The initial random fields are generated according to the procedure given by Rogallo [66]. The initial velocity field is expressed in terms of its Fourier coefficients of the components as

\[ \hat{u}(k_1, k_2, k_3) = \left( \frac{k_2}{k_{12}} a + \frac{k_1}{k_{12}} k_3 b, \frac{k_2}{k_{12}} k_3 b - \frac{k_1}{k_{12}} a, -\frac{k_1}{k_{12}} a, -\frac{k_2}{k_{12}} b \right) \]  

(6.13)

where \( k_i \) are the wave numbers, \( k = \sqrt{k_1 k_2} \) is the wavenumber magnitude, and \( k_{12} = \sqrt{k_1^2 + k_2^2} \).

In the special case of \( k_{12} = 0 \) we define \( \frac{k_1}{k_{12}} = 0 \) and \( \frac{k_2}{k_{12}} = 1 \). The quantities \( a \) and \( b \) are

\[ a = \sqrt{\frac{2E(k)}{4\pi k^2}} e^{i\phi_1} \cos(\phi_3), \quad b = \sqrt{\frac{2E(k)}{4\pi k^2}} e^{i\phi_2} \sin(\phi_3) \]  

(6.14)
where \( \phi_1, \phi_2 \) and \( \phi_3 \) are random numbers uniformly distributed on \([0, 2\pi)\) and \( E(k) \) is the energy spectrum. The \( \text{rms} \) velocity can be defined as

\[
\mathbf{u}_{\text{rms}} = \sqrt{\frac{1}{3} \sum_{i=1}^{3} (u_i)^2}
\] (6.15)

where \( \langle ... \rangle \) is a volume average over the computational domain at a fixed time instant. Turbulent kinetic energy or TKE can be defined as the integral of the energy spectrum over all wave numbers and has the following relation with the \( \text{rms} \) velocity

\[
\text{TKE} = \int_{0}^{\infty} E(k) dk
\] (6.16)

We define the Taylor microscale \( \lambda \) and the Taylor Reynolds \( \text{Re}_\lambda \) number as

\[
\lambda^2 = \frac{\mathbf{u}_{\text{rms}}^2}{\langle \left( \frac{\partial u_1}{\partial x_1} \right)^2 \rangle}, \quad \text{Re}_\lambda = \frac{\mathbf{u}_{\text{rms}} \lambda \langle \rho \rangle}{\langle \mu \rangle}
\] (6.17)

The turbulent Mach number and \( \text{rms} \) Mach number are defined as

\[
M_t = \frac{\sum_{i=1}^{3} (u_i)^2}{\langle c \rangle}, \quad M_{\text{rms}} = \left( \frac{\sum_{i=1}^{3} (u_i)^2}{c^2} \right)^{1/2}
\] (6.18)

### 6.3.2.2 Simulation of Subsonic Compressible Turbulence

In this section, we focus our attention on the simulation of a low \( \text{rms} \) mach number case of compressible isotropic turbulence. The main motivation for this simulation is to validate the performance of the code and verify our results in comparison to published data in the...
literature. We use the setup of the case IDC96 which was modeled in Blaisdell et al. The initial velocity spectrum is a top hat which has non-zero contributions in the wavenumber range of $8 \leq k \leq 16$. The initial density, pressure, and temperature fields are uniform and the velocity fluctuations are purely solenoidal. The initial velocity and thermodynamic fields are obtained on a uniform grid from the Fourier coefficients using a fast Fourier transform which generates a flow field correlated according to the top hat spectra. The initial conditions on the computational domain is then obtained using an interpolation from the Fourier grid to the Gauss points.

Case IDC96 has an initial Mach number of $M_t = 0.3$, an initial turbulent Reynolds number of $Re_T = 160$ and an initial Taylor Reynolds number of $Re_\lambda = 40$. The reference simulation was performed with a Fourier spectral method with $96^3$ grid points. In order to validate the performance of our code, we simulate the same case using 6 $P15$ elements in each spatial direction. This constitutes a mesh comprising of $(6 \times (15 + 1) = 96)^3$ Gauss solution points which provides an exact same resolution as the reference IDC96 simulation.
Figure 36 shows comparisons of energy and dissipation spectra between results obtained by DSEM and the reference DNS results of Blaisdell et al. [65]. It is observed that the DSEM code is clearly capturing the general shape of the spectra although we see some small deviations at low wave numbers. The behavior of the high-frequency part, underscores the accurate capturing of high-wave number eddies in the flow field which has a greater importance. In numerical simulation of turbulence, the behavior of small turbulence structures are usually governed by numerical errors. However, in a high-order method, like DSEM with very small dissipation and dispersion error, the numerical errors do not accumulate and as a result the resolution of small
scale turbulence is more accurate. Comparison of the turbulence kinetic energy decay rate, as shown in Figure 37 also confirms the accuracy of the simulation.

![Figure 37: Decay of turbulent kinetic energy for isotropic turbulence](image)

6.3.2.3 Simulation of Supersonic Compressible Turbulence

The actual test case is that of decaying isotropic turbulence with a relatively high \( \text{rms} \) Mach number which generates eddy shocklets. Given sufficiently high turbulent Mach number and Turbulent Reynolds number, shock waves develop spontaneously from the turbulent motions. These shocklets are distributed randomly within the computational domain and this very character of the problem can serve as a good test to measure the ability of the numerical scheme to
dynamically locate and resolve these shock waves. In addition, the numerical method should be capable of preserving the accuracy for broadband motions in the presence of shocks.

In the specific problem setup considered here; the initial velocity fluctuations, $u_{i,0}$ are purely solenoidal and have the following spectrum in the wavenumber space

$$E(k) = Ak^4e^{-2k^2/k_0^2} \tag{6.19}$$

where $k$ is the wave number, $k_0$ is the wave number at which the spectrum peaks, and $A$ is a constant chosen to get a specified initial kinetic energy. As it can be found in the literature, this specific problem suffers from a start-up issue \[67\]. Before amplitude-phase correlations develop from the initial uncorrelated random field, the flow undergoes a fast transient during which the divergence of the velocity increases rapidly accompanied by large negative values of the velocity derivative skewness. This might be crippling in the beginning of the simulation and a careful initialization strategy should be devised. A simple strategy is to initialize the simulation with no fluctuations of any thermodynamic quantity.

For the specified velocity spectrum in Equation 6.19 it can be shown the turbulent kinetic energy and the initial large eddy turn over time $\tau$ are given by

$$TKE = \frac{3A}{64}\sqrt{2\pi k_0^5}, \quad \tau = \sqrt{\frac{32}{A}(2\pi)^{1/4}k_0^{-7/2}} \tag{6.20}$$
which can be related to the \textit{rms} velocity as

\[ TKE = \frac{3u_{rms}^2}{2} \] (6.21)

now by specifying parameters \( A, k_0, M_t \) and \( \text{Re}_\lambda \) and using Equation 6.17, Equation 6.18 and Equation 6.20, the initial condition can be setup. Here, we use the set of initialization parameters which are extracted from [68]. The details of this case are provided in Table 1.

<table>
<thead>
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<th>( \text{Re}_\lambda )</th>
<th>( M_t )</th>
<th>( A )</th>
<th>( k_0 )</th>
</tr>
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<tbody>
<tr>
<td>100</td>
<td>0.6</td>
<td>0.01246</td>
<td>4</td>
</tr>
</tbody>
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In this the initial density is \( \rho_0 = 1 \) and the initial Taylor microscale is \( \lambda_0 = 2/k_0 = 0.5 \). The initial Mach number is high enough for the flow to spontaneously form shocklets and the Reynolds number is high enough to have a broad range of scales for vortical motions. Eddy shocklets activate the shock-capturing mechanism and if the method is not capable of adding localized and proper dissipation significant errors can occur. Since the initial conditions are not in acoustic equilibrium, a field of background acoustic waves develops and persists throughout the simulation. Similarly, there are initial entropy modes and a problem with large acoustic and entropy modes is desirable here since it can make the numerical scheme more challenged.
The simulation is performed on a $16^3 \mathcal{P}5$ element mesh (equivalent of a mesh with $96^3$ nodes) which spans $[0,2\pi]$ along each axis in the physical domain. The simulations are run for 4 eddy turn over times, i.e. $t/\tau = 4$. Figure 38 shows the 3-dimensional plots of $rms$ velocity at the initial and final simulation times and we can observe the decay of turbulence in a qualitative sense. Similarly, ?? shows the plots of Mach number at initial and final simulation times. As it can be seen from the plots of Mach number, we can see supersonic patches (in red) in the beginning of the simulations which is a good indication of shocklets formation. Results are compared quantitatively against the reference solution from the DNS on a $256^3$ grid from Johnsen et al. [69]. We have run two sets of similar simulations with the original EV method which indicates the EV method without the modifications introduced at the beginning of this chapter and a also with the modified EV method.
Figure 38: 3D plots of \( \text{rms} \) velocity at \( t/\tau = 0.0 \) and \( t/\tau = 4.0 \)
Figure 39: 3D plots of local Mach number velocity at $t/\tau = 0.0$ and $t/\tau = 4.0$
The temporal evolution of the mean-square velocity and the variance of the density are plotted in Figure 40. While the modified EV method agrees well with the reference solution, the original EV method under-predicts the temporal behavior of the turbulence kinetic energy and density variance indicating its dissipative behavior. The energy spectra at the final time is displayed in Figure 41 which shows the spectra obtained using the original and modified EV method in comparison with the spectra from the reference simulation. While the results obtained using the modified EV method are in good agreement with the DNS results, the original EV method appears to be too dissipative and the obtained energy spectra shows good agreement with the reference solution for a small range of wavenumbers only.
Figure 41: Energy spectra for original and modified EV method at $t/\tau = 4.0$
CHAPTER 7

CONCLUSIONS

7.1 Broad Impact of Research

Improved design of advanced propulsion systems and high-speed flight vehicles rely heavily on the detailed understanding of supersonic compressible flows. High-fidelity numerical simulations can play an important role in unraveling the associated complex flow physics. The broad impact of the current research is delivery of a computational tool for simulation of supersonic compressible flows often characterized by the concurrent presence of shock waves and turbulence.

Particular focus has been on the development of an efficient and easy to implement shock capturing scheme for high-order methods. We used a discontinuous Galarkin spectral element method because of its high spatial and temporal accuracy, flexible meshing and ease of boundary condition and parallel implementation. On the contrary, this numerical method is still young and has had limited use in practical engineering application especially for supersonic flows. This research was aimed at developing a cutting-edge numerical technique which combines the desirable features of high-order discontinuous Galerkin methods with an efficient and robust high order shock-capturing and stabilization procedure to be used for the simulation of high-speed turbulent and shock dominated flows.
The first part of our research extends the use of the original entropy viscosity method \cite{46} to high-order discontinuous collocation methods. In order to achieve a smooth artificial viscosity distribution, a combination of explicit filtering and smoothing for solution values and entropy viscosity associated fluxes is used. The resulting method has two main advantages compared to its counterparts. First, it makes a clear distinction between shocks and contact discontinuities and adds substantially less viscosity at the location of contact discontinuity thus enabling a sharp resolution of the contact surface. Second, it produces a smooth variation in artificial viscosity, which allows the use of high-order elements without being troubled with oscillations at the element interfaces. Using high-order elements allows us to run a simulation with a certain number of solution points with less number of elements which drastically reduces the computational cost.

In the second part, we presented a modified version of our shock capturing method for simulation of viscous flows. A special consideration is given to turbulent flow and further refinement is conducted to make the method more suitable for supersonic turbulence simulation. The modified method retains the shock capturing capability of the original formulation while significantly improving performance in terms of acoustic motions and thermodynamic fluctuations for high Mach number turbulence. Stabilizing the shocked turbulent flow is demonstrated by simulating the decaying isotropic turbulence with relatively high turbulent mach numbers. The obtained results confirm the ability of the modified method to capture shocklets while preserving the main features of the turbulence structure which is, in large part, due to minimal dissipation added to turbulent structures.
7.2 Future Work

The dissertation has been a part of a larger research effort to develop accurate and affordable computational tool for the simulation of reacting turbulent flows in supersonic combustors. In this research foundation of a high-order shock capturing method for the simulation of supersonic cold flow has been successfully laid down. However, performing further analysis and numerical tests seems inevitable in order to make this method usable for reacting flow simulation in a supersonic combustion chamber. To make the method capable of shock capturing in reacting flow where there are multiple species and also additional source terms in the momentum and energy equations, one should make some modifications in the EV formulation. First and foremost, the entropy residual should be updated reflecting the effect of the heat release source term in the energy equation as it has a direct effect in the entropy balance equation. Secondly, new artificial diffusivities should be introduced for the specie transport equations as they will be sensing a discontinuity wherever the flow passes through a shock.

On the fundamental research side, the method has a potential to be used as an interface tracking scheme for multiphase flow applications. A simple example was presented in Chapter 5 for the Rayleigh–Taylor instability problem and this capability was briefly touched upon, however exploring its full potential requires more investigation.
APPENDIX

Some of the art work and material found in Chapters 5 had been previously published by Elsevier publications as a journal articles. The publisher policy allows using those material in a thesis or dissertation written by journal’s primary author. A copy of the publisher’s policy can be found below. For more information please go to: http://www.elsevier.com/journal-authors/author-rights-and-responsibilities#author-use/

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