COMPUTATION OF 2D INVISCID COMPRESSIBLE FLOW USING AN ENTROPY CONSISTENT EULER FLUX

by

NUR KHAIRUNNISA HANISAH BINTI ROSLAN

Thesis submitted in fulfilment of the requirements
for the Degree of
Master of Science

July 2013

ACKNOWLEDGMENTS

In the name of Allah, Most Gracious, Most Merciful. Thankful to Him that after going through various twists, with the blessing and His willing, I've finally managed to complete the research and this thesis.

First and foremost, I would like to express my gratitude to my beloved husband, Mohd Suhairie Hanif for his love and endless support. Without him, I might not be able to bear this burden alone. Thank you for waiting for me patiently. Also thank you to my dearest father, Roslan Noordin for being very supportive and always been behind me from the first day I decided to pursue my study and also for showing me the way when I hesitate. Also not forgetting, thanks go to my mother, Faridah Johan for her support in reducing the burden borne by me and to my siblings that always rely on their big sister to finish this journey with flying colours. Your prayers make these dreams into reality. Alhamdulillah.

In this opportunity, I would like to express my gratefulness to my supervisor, Dr Farzad Ismail, who works tirelessly to help and support me until the end. Thank you for always inspiring me to finish my studies. Also for the confidence and trust bestowed because it gave me the strength to face the pressure to complete this research. Thank you also to accept me as your student and devote knowledge of CFD that has become increasingly attractive and make me more interested in the field of numerical codes. It is an incredible journey and also thank you for the financial support during my work as a research assistant under your grant.

I also would like to thank to all my colleagues especially to my backbone in this research, Shalihatun Azlin for her support for me to complete this study. It was very tough in the beginning but she always there for me to provide guidance especially in knowledge of C++. Even though we know each other for only four years, the quality time we shared will be my fondest memories forever.

Last but not least, I would like to thanks to School of Aerospace Engineering staff and everyone involved either directly or indirectly in completing this research. This research would not succeed without the support and help from you all.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LISTS OF ABBREVIATIONS

1D	One-Dimensional
2D	Two-Dimensional
3D	Three-Dimensional
AoA	Angle of Attack
AUSM	Advection Upstream Splitting Method
CFD	Computational Fluid Dynamics
CFL	Courant-Friedrichs-Lewy condition
CV	Control Volume
DES	Detached-Eddy Simulation
EC	Entropy Consistent Euler Flux
EFD	Experimental Fluid Dynamics
ENO	Essentially Non-Oscillatory
FCT	Flux-Corrected Transport
FDM	Finite Difference Method
FDS	Flux Difference Splitting
FEM	Finite Element Method
FVM	Finite Volume Method
FVS	Flux Vector Splitting
GCI	Grid Convergence Index
IDE	Integrated Development Enviroment

LES	Large Eddy Simulation
MUSCL	Monotonic Upwind Scheme for Conservation Laws
NS	Navier-Stokes
PDE	Partial Differential Equation
RANS	Reynolds Average Navier-Stokes
RHS	Right Hand Side
RK3	Third-order Runge-Kutta method
SWS	Steger-Warming Splitting
TVD	Total Variation Diminishing
VLS	Van Leer Splitting
V&V	Verification & Validation
WENO	Weighted Essentially Non-Oscillatory

NOMENCLATURE

Symbol	Description
a	Speed of sound
A	Cell area
$\mathbf{A}$	Jacobian matrix
AR	Aspect ratio
$C0$	Computed cell
$C1, C2, C3, C4$	Neigbouring cells
C_G	Correction factor
C_p	Pressure coefficient
$\mathbf{D}$	Dissipation matrix
e	Fluids internal energy
$E1$	Edge at particular face
E	Total energy
EQ	Equiangular skew
E_{exact}	L1-Norm between numerical and analytical solution
E_{exp}	L1-Norm between numerical and experimental solution
$\mathbf{f} = (\mathbf{f}_x, \mathbf{f}_y)$	Conservative flux vectors
$\mathbf{F}$	Net flux at cell interface
F_s	Safety factor
H	Total enthalpy

$\mathbf{L}$	Left eigenvector matrix
Ma	Mach number
$\mathbf{n} = (n_x, n_y)$	Normal vector
P_G	Theoretical spatial order of accuracy
q	Normal velocity
r	Tangential velocity
r_G	Grid refinement ratio
$\mathbf{R}$	Right eigenvector matrix
R_G	Grid convergence ratio
S	Physical entropy
$\mathbf{S}$	Diagonal scaling matrix
$\mathbf{t} = (t_x, t_y)$	Tangent vector
$\mathbf{u}$	Conservative variables-vector
U	Entropy function
U_G	Grid uncertainty of grid refinement
U_{SN}	Numerical solution uncertainty
U_V	Validation uncertainty
$\mathbf{v}$	Entropy variable-vector
$V1, V2, V3, V4$	Vertices around a cell
$\mathbf{w}$	Primitive variables-vector
$\nabla\mathbf{W}$	Slope gradient

Greek

γ	Fluids specific heat ratios
δ	Percentage difference of L1-Norm at ($\Delta x =$ zero) w.r.t. the reference value (origin)
ϕ	Slope Limiter
λ	Fluids wave speeds
Δs	Cell face length
Δt	Time step
Δx, Δy	Mesh increment in (x, y)-axis
$\mathbf{\Lambda}$	Diagonal eigenvalue matrix

Subscripts

c	(x, y) coordinates of cell centroid
f	(x, y) coordinates of cell interface
i	Index of computed cell
j	Index of neigbouring cells
L	Left cell interface
R	Right cell interface

Superscripts

n	Discrete time level
$\bar{}$	Arithmetic mean
ln	Logarithmic mean

PENGIRAAN DUA DIMENSI BAGI ALIRAN MAMPAT TIDAK LIKAT MENGGUNAKAN FLUKS ENTROPI EULER KONSISTEN

ABSTRAK

Fungsi Roe fluks merupakan salah satu fungsi fluks yang paling mantap bagi aliran tak likat dan digunakan secara meluas dalam pengkodan perkomputeran dinamik bendalir (CFD). Walau bagaimanapun, didapati bahawa fluks Roe mengalami ketidakstabilan kejutan sepertimana yang sering dicerap ketika kejutan yang sangat kuat seperti yang berlaku di dalam aliran hipersonik. Ini mungkin kerana fluks Roe tidak mematuhi hukum termodinamik kedua yang mana ia adalah kritikal dalam penangkapan kejutan. Fluks Euler Entropi konsisten (EC) merupakan kaedah baru bagi menangkap kejutan yang dibangunkan oleh Ismail & Roe dalam usaha untuk mengatasi kekurangan fluks Roe. Fluks EC ini direka secara diskret untuk memenuhi hukum pengabadian asas yang secara diskret mematuhi hukum termodinamik kedua (pengawalan entropi). Namun begitu, kajian terdahulu mengenai skim-skim entropi adalah berasaskan masalah ujian akademik dalam satu dimensi (1D) sahaja.

Objektif utama kajian ini adalah bagi menentukan sama ada prestasi fungsi fluks EC relatif kepada fluks Roe dalam beberapa kes-kes ujian masalah kejuruteraan termasuk subsonik, transonik, aliran supersonik dan hipersonik. Fungsi fluks baru telah diuji untuk masalah ujian 1D dan 2D. Masalah ujian 1D berdasarkan masalah tiub kejutan Sod sedangkan masalah 2D termasuk aliran Mach 3 ke atas tangga, aliran mantap ke atas silinder dan aliran mantap ke atas aerofoil NACA 0012. Untuk penyelesaian masalah 1D dan 2D ini, satu kod penyelidikan CFD yang berasaskan aliran boleh mampat tak likat telah berjaya dibangunkan khusus untuk geometri 2D umum garis melengkung yang menggunakan grid berstruktur. Grid

ini dijana menggunakan perisian GAMBIT dan kemudian dimasukkan ke dalam perisian penukar hasilan sendiri bagi memastikan bahawa konfigurasi grid tersebut adalah bersesuaian dengan penyelesai CFD baru dibangunkan ini.

Ujian kesahan dan penentusahan (V & V) telah dijalankan bagi menentukan ketepatan dan ketidakpastian kod dan grid yang digunakan dalam penyelidikan ini. Secara ringkas, hanya kaedah tertib pertama sahaja yang disah dan ditentusahkan tetapi tidak dilaksanakan dalam kaedah tertib kedua. Berdasarkan aliran mantap tak likat ke atas silinder, ketepatan kaedah tertib pertama adalah sekitar (0.42%) dengan maksimum ketidakpastian sebanyak (0.42%). Secara keseluruhannya apabila menghadapi kejutan yang sangat kuat, fungsi fluks baru ini menghasilkan keputusan yang lebih baik daripada fluks Roe yang lazimnya menghasilkan satu penyelesaian tidak fizikal. Bagi masalah-masalah lain seperti aliran subsonik rendah, subsonik dan transonik melalui suatu silinder dan aerofoil, fluks Roe memang diketahui menghasilkan penyelesaian yang cemerlang dan didapati fluks EC juga sebanding dalam menghasilkan keputusan tepat relatif dengan fluks Roe. Ini mungkin menunjukkan fluks EC mempunyai skop yang lebih luas bagi aplikasi CFD dalam aliran boleh mampat berbanding fluks Roe.

COMPUTATION OF 2D INVISCID COMPRESSIBLE FLOW USING AN ENTROPY CONSISTENT EULER FLUX

ABSTRACT

The Roe flux function is one of the most established flux functions for inviscid flow and widely used in many CFD codes. However, the Roe flux suffers from shock instability which is usually observed for very strong shocks as in hypersonic flow. This maybe because the Roe flux does not strictly adhere to the second law of thermodynamics which is critical to capture shocks. The entropy consistent Euler flux (EC) is a new shock capturing method developed by Ismail & Roe in an attempt to overcome the above mentioned deficiencies of the Roe flux. The EC flux is designed to discretely satisfy the basic conservation laws, besides satisfying the second law of thermodynamics (entropy control). Most of the previous studies on the entropy schemes are based mainly on academic test problems using one-dimension.

The main objective of this study is to determine the performance of the EC flux function relative to the Roe flux under subsonic, transonic, supersonic and hypersonic flow. This new flux function is tested for 1D and 2D test problems. The 1D test problem is based on Sod's shock tube problem, whereas the 2D problems include the Mach 3 flow over a staircase, a steady flow over a cylinder and a steady flow over a NACA 0012 airfoil. In order to solve these 1D and 2D problems, an in-house CFD research code based on inviscid compressible flow was developed for a general 2D curvilinear geometry using structured grids. The grid is generated using GAMBIT software and then fed into a self-written converter software to ensure that the grid configurations are compatible with the newly developed CFD solver.

Validation and verification (V&V) exercises is carried out to study the accuracy and uncertainty of the code and grids used in this work. Briefly, only the first order method is validated and verified but not the second order method. Based on the steady inviscid flow over a cylinder, the accuracy of the first order method is about (0.42%) with a maximum uncertainty of (0.42%). Overall the new flux function produced better results than the Roe flux when dealing with very strong shocks where the latter usually produced an unphysical solution. For other problems such as the low-subsonic, subsonic and transonic flow pass a cylinder and airfoil where the Roe flux is known to produce excellent solutions, the EC flux produces comparably accurate results relative to the Roe flux. This perhaps indicate the EC flux has a wider scope of CFD application in compressible flow compared to the Roe flux.

CHAPTER 1

INTRODUCTION

1.1 Introduction

We are surrounded by fluids, and fluids are involved in most phenomenon in this world, regardless of time and place. For example, when breathing, the air is inhaled into the lungs and oxygen that enters the bloodstream will travel to the heart. Fluids cover more than 60% of the human body which includes in blood, brain, muscles and bones. Fluid flow enable us to fly planes, sail boats and parachuting. There are a lot of disciplines involving fluid flow, including aerospace, automotive, electronics, chemicals and many more. Thus, the fluid flow behaviour is essential to be observed for researchers, engineers, mathematicians and physicists. Quantitative and qualitative observations can give a clearer understanding on how the fluids behave.

Simple problems can be solved analytically but when it involves complex problems such as high-speed aircraft or fluid flow within human body (blood vessels, fluid within brain), it is impossible to solve it analytically. An alternative approach needs to be considered. Computational fluid dynamics (CFD) was introduced in early 1960s to overcome these difficulties. CFD is the science of predicting physical fluid flow in specified circumstances by solving the governing mathematical equations using numerical process. Computers are used to perform the mathematical calculations and simulate the fluid interaction. It covers a wide range of applications such as, simultaneous flow of heat, mass transfer and chemical reaction. One of the benefits of CFD is that it allows engineers to optimize the engineering design products and reduce the potential chances of product failures. Meanwhile, in research, CFD can provide a broad understanding in a particular field.

1.2 Introduction of CFD

The Navier Stokes (NS) equations are the fundamental basis of almost all CFD problems since the equations are based on real fluid conditions which include conservation principles, viscous flow and heat transfer and often are used for solving turbulent flow. There are many examples of modelling approximation of turbulence effects such as Reynolds Averaged Navier-Stokes (RANS) (Reynolds, 1895), Large Eddy Simulation (LES) (Smagorinsky, 1963), and Detached-Eddy Simulation (DES) (Travin et al., 2004) in order to predict the turbulent flows.

It is not practical to solve the full NS equations when viscous effects are not dominant particularly in the inviscid region of high Reynolds number flow. Thus, the simplified NS equations which excludes viscous effect called Euler equation is introduced. The Euler equations are based on fully inviscid flow solving waves and high speed flow, e.g. shock waves and sonic waves. The research areas which utilize inviscid flow as the main focus include compressible flow, aerodynamics and rocket propulsion.

Basically CFD is used to simulate engineering problems which are based on physics and are modeled through a set of mathematical equations. These mathematical models are a set of partial differential equation (PDE) which must be discretized. Once discretized, these mathematical models would be numerically solved and the results can be visualized through a plotting software.

1.3 Second Law of Thermodynamics

In this research, the Euler equation is used as the model equation for solving inviscid compressible flow. The Roe flux function is one of the most established flux functions for inviscid flow and widely used in CFD code such as Fluent, STAR-

CD and other industrial and research codes. However, Roe flux (Roe, 1981) suffers from shock instability such as the carbuncle phenomenon, which is usually observed for a very strong shock as in hypersonic flow (Quirk, 1994). This is perhaps because the Roe flux does not strictly satisfy the second law of thermodynamics which is crucial in shock capturing.

Strictly speaking, entropy should not be produced for continuous flow. Yet most, if not all numerical schemes in CFD will generate spurious (artificial) entropy for smooth flows. Usually a test of a good CFD method or code is that it produces minimum entropy for continuous flows and this is rarely met even for simple flows. On the other hand, for a discontinuous flow such as flow across a shock, entropy should be produced not only with the proper sign but also with the proper amount. The flux function that is proposed in this study satisfies the basic conservation laws (mass, momentum and energy) and precisely satisfying the two laws of thermodynamics, particularly the second one which is in controlling the amount of entropy being generated.

1.4 Problem Statements

As mentioned earlier, the Roe flux is used in most commercial CFD softwares. Therefore, perhaps the software solutions are not reliable for high speed flows. To overcome the disadvantage of Roe flux which only consider the first law of thermodynamics, (Roe, 2006),(Ismail and Roe, 2009) had developed a new flux function that adheres to the second law of thermodynamics. The new flux function is not expensive and is comparable in cost relative to the Roe flux. The new flux function called the entropy flux function (EC) has been tested for one-dimensional (1D) test problems for scalar and system problems and successfully produced good results and accurate entropy production across a shock. The EC flux can be a good candidate for replacing the Roe flux in the future.

However, the EC flux has only been tested for 1D problems. The new flux function has not been tested on two-dimensional (2D) complex test problems, specifically on the complex test problem related to engineering. In this work, 2D EC flux has been evaluated by applying it over several engineering test cases such as circular cylinder and NACA airfoil.

1.5 Research Objectives

The main purpose of the work described here is to demonstrate that the new flux function is more reliable than the Roe flux when dealing with high-speed flow. Referring to the problems stated in Section 1.4, the specific aspects of the approach developed in this research are as follows:

1. To develop an in-house CFD code for 1D and extension to 2D.
2. To determine the performance of the new flux function in 2D cases compared to the Roe flux in several test cases which include subsonic, transonic and supersonic flows.
3. To verify and validate the in-house CFD code.
4. To design a grid generation code function to extract mesh from commercial grid generator software and to be used in the in-house CFD code.

1.6 Scope of Research

The application of the new flux function on 2D test problems is only a preliminary study. Thus, the Roe flux alone is sufficient as the benchmark for 2D study since the Roe flux is a well-established flux function which has been widely used in many commercial CFD softwares. Thus, restricting only to the Roe flux has greatly reduced the time consumed in completing this research.

The other limitation in this research is that the complex geometries of 2D test problems are based on quadrilateral grids created by a commercial grid generator software. The grid quality from the commercial software are usually quite good hence reducing the possibilities of grid errors that may contribute to the results. This is to ensure that the results produced from the code solver are mainly based on the flux function and the code.

1.7 Thesis Outline

In this study, a numerical code written in C++ is developed for solving aerospace fluid dynamics problem. Most of aerospace problems deal with a slender body at high Reynolds number which involves thin boundary layer around the body. Inviscid calculations are expected to be accurate when the flow is outside the boundary layer. There are limitations for inviscid flow calculations in the sense that the predicted drag coefficients are inaccurate due the skin friction terms being neglected. For a start, only the inviscid terms are accounted for in the code leaving out the viscous effects of the fluid which greatly simplifies the code development process since turbulent flow can be ignored at this stage.

This thesis is organized in 5 chapters. Chapter 1 presents the introduction to the work. The rational for carrying out this work, its objectives, scope are also presented.

Chapter 2 will explore the literature that is relevant to understanding the development of, and interpreting the results of this study. The first two parts of the literature review will discuss two types of capturing scheme: classical and modern capturing schemes. The third part of the literature review is a summary of research on second law of thermodynamics and numerical schemes that are entropy stable and consistent.

Chapter 3 presents the details of research methods used in the study; to develop a complete code of numerical schemes. There are three main stages in the development of the proposed scheme; pre-processing, processing and post-processing. The pre-processing stage is an initial setup of test problems before the solver performs the computation, whereas the processing stage is where the numerical scheme has been constructed and the main computation begins. Finally the code's accuracy and uncertainty is checked through Verification and Validation (V&V) assessments in post-processing stage.

In Chapter 4, the results and discussions are presented. This chapter will also be the demonstration of results between the new flux and the Roe flux. The results are compared qualitatively and quantitatively.

Lastly, a summary of the research is presented in Chapter 5. This chapter also gives some concluding remarks and comments concerning proposed future work.

CHAPTER 2
LITERATURE REVIEW

2.1 Introduction

There are two types of flow in CFD which are incompressible flow and compressible flow. Both incompressible and compressible flows are determined by the speed of the flows or the speed of moving object through fluid flow. The Mach number, (Ma), is a dimensionless unit to represent the ratio of speed of the flow over the local speed of sound and is widely used by the CFD community to classify flows for ages. The flow is estimated as incompressible when the Mach number of the flows is below 0.3 whereas the compressible flow is when Mach number is 0.3 and greater.

Incompressible flows are an approximation to simplify the complexity of compressible flows. When some volume of fluid flow transfer from one location to other, the quantity of the fluid called density will either increase or decrease due to a pressure change. When velocity of the flow is relatively small, the pressure will not change excessively. This means that the volume is preserved during the fluid transition and the density does not vary much and such flows are categorized as incompressible flows. This approach is generally adopted in majority of the studies conducted in turbulent flow. These turbulence studies are quite extensive which include smoke around objects [(Fedkiw et al., 2001), (Lentine et al., 2010)], dam break (Biscarini et al., 2010), and blood flow (Behbani et al., 2009).

Unlike incompressible flow, compressible flow represents a more realistic fluid flow. There are four speed regimes for compressible flow. The regimes can be loosely defined as subsonic flow ($0.3 \leq Ma < 1$), transonic flow ($Ma = 1$), supersonic flow ($1 \leq Ma < 5$) and hypersonic flow ($Ma \geq 5$). Shock waves occur in compressible flow due to the sudden change in its thermodynamic properties spanning a very short distance. In general, these shocks usually occur when the flow is either supersonic or hypersonic.

2.2 Shock Wave

Three types of nonlinear waves are present in compressible flow; rarefactions, shocks and contact discontinuities in 1D. In 2D there is the shear wave. Rarefaction wave describes fluids expansion from high pressure to low pressure. In this case, the density and pressure of the fluid will gradually decrease with time and space. The rarefaction wave is a continuous flow while shocks and contact discontinuities are sudden variable jumps in the flow causing flow discontinuities. The contact discontinuity is a partially discontinuous flow due to the occurrence of density jump, other variables such as pressure and velocity are continuous. When two gases collide with each other, one experiences a shock, while the other undergoes expansion. When the two gases meet, they are separate by contact.

A shock wave is a very thin layer of a sudden change in density, temperature, entropy and speed (Ziniu et al., 2013). A shock happens when wave propagates faster than speed of sound which means the wave travels at Mach number higher than one. Thus all of the information about the incoming high speed wave reach the surrounding fluids too abruptly. Unaware of the incoming wave, the surrounding fluids have little time to adjust leading to collision of gas molecules between the incoming wave and the surrounding fluids. The collision causes an abrupt change of gas properties. The types of shock wave phenomena that commonly occur are sonic booms created by supersonic jet, bow shocks from flying bullets, and also in natural occurrences such as in tsunami and thunder created by lightning.

It is important to study shock wave in advanced aerospace engineering technology especially involving supersonic/hypersonic vehicle either aircraft or spacecraft. This is because shock waves can harm people and environment if not well treated and also drastically degrades aerodynamic performance of aircrafts. The effects of shock waves are very challenging to be analyzed in the real world. Thus, high speed wind tunnel for laboratory experiments is designed to overcome the problems [(Lilley, 1948), (Huntsberger and Parsons, 1954), (Silva et al., 2009)]. Laboratory experiments on scale model known as Experimental Fluid Dynamics (EFD) produce reliable data because it measures actual conditions, unlike computation where values are predicted. Unfortunately, there are severe limitations to the wind tunnel application. The costs to build high speed wind tunnels are expensive in terms of the wind tunnel size and requires a large power supply to produce supersonic/hypersonic flow. In addition, test objects need to be manufactured first and they are not easily modified for changing test configurations.

Since the last 30 years, numerical approach has been adopted by several researchers to solve flow with shocks in a more efficient way [(Godunov, 1959), (Harten, 1983), (Salas, 1976)]. Numerical techniques are flexible for complex geometries and economical because it only needs a good numerical code and a decent computer to run the numerical experiments. Of course, numerical results alone are not reliable enough because it is only an approximation. Thus laboratory experimental results are still used to benchmark numerical experiments. One of the most prominent numerical techniques to capture shock in CFD is the shock capturing scheme.

2.3 Shock Capturing Scheme

Shock-capturing schemes are widely used techniques for computing flows with shocks. The numerical schemes are designed using three steps; (1) choose an appropriate mathematical model, (2) choose a suitable discretization method to discretize the mathematical model, and (3) decide the suitable discretization type. Shock capturing schemes are based mostly on the inviscid Euler equations, a system of hyperbolic conservation laws which admit discontinuous flow. The one-dimensional Euler equations in conservative form are

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}_x}{\partial x} = 0 \tag{2.1}$$

where the conservative variables are mass, momentum and energy, defined as $\mathbf{u} = [\rho \quad \rho u \quad \rho E]^T$ and conservative flux, $\mathbf{f}_x = [\rho u \quad \rho u^2 + p \quad \rho u H]^T$. The total energy is defined as $E = e + \frac{u^2}{2}$ and the total enthalpy $H = E + \frac{p}{\rho}$. The compatibility relation between pressure and fluid internal energy, e, is used for closure $p = \rho e(\gamma - 1)$ where γ is the gas specific heats ratio for ideal gas.

There are three popular discretization methods; (1) Finite Volume Method (FVM), (2) Finite Element Method (FEM) and (3) Finite Difference Method (FDM). The FVM is widely regarded to be the most suitable discretization method to compute flows with shocks in engineering problems [(Hubbard and Garcia-Navarro, 2000), (Qiu and Shu, 2002)]. The FVM is based on the integration of the governing equation that will guarantee conservation of physical quantities such as mass, momentum, energy. The FVM subdivides the flows into a finite number of computational cells called control volume (CV). The computational nodes are located at the centroid of CV and the fluid properties are conserved within each CV.

The FEM is similar to FVM because this method also uses integral method. The difference between FEM and FVM is that FEM uses polynomial weighting function whereas FVM only uses a constant weighting function. Thus, FEM is usually more complicated but more accurate relative to FVM and not suitable for long simulations of complex engineering problems.

Unlike the other two methods, FDM is based on the differential form of the equations. FDM is the least suitable discretization method to capture shocks because FDM approach is not mathematically well-posed when predicting a discontinuous profile although it is quite accurate for continuous flow. It is also less flexible for irregular domains since it usually involves conformal mapping grids to map from Cartesian grids to irregular grids.

The last step is to choose the type of discretization in CFD. The most commonly chosen discretization types to design numerical shock capturing schemes are central discretization and upwind discretization. Thus, there are two categories of shock capturing scheme; (1) classical shock capturing schemes based on central discretization, and (2) modern shock capturing schemes based on upwind discretization, (Chen, 2001).

2.4 Classical Shock Capturing Schemes : Central

Classical capturing methods use central discretization technique which do not require the explicit knowledge of the characteristics of the system. Examples of well known classical shock capturing scheme are the Lax-Wendroff scheme, the Beam Warming scheme, and the McCormack scheme.

The central or symmetric discretization makes the classical shock capturing scheme a second order accurate scheme without applying additional techniques. The classical shock capturing scheme has an advantage for not being dissipative thus produce accurate results in smooth and weak shock solution. However, they are prone to generating spurious oscillations across strong shocks in the solutions on account of not producing enough numerical dissipation. Mathematically, this is because the method violates Godunov theorem.

2.4.1 Addition of Artificial Diffusion for Classical Capturing Scheme

In order to overcome the spurious oscillations across strong shocks, the classical capturing scheme is remedied by adding a limited amount of diffusive flux to the scheme. In this approach, the artificial diffusion is tuned to introduce enough dissipation near discontinuities but made small enough to be negligible in smooth regions. However, the difficulty with this approach is that it is hard to determine the amount of dissipation needed without causing unnecessary smearing.

2.5 Modern Shock Capturing Schemes : Upwind

The upwind discretization uses wave propagation information as the basis of its numerical design (Chen, 2001). If the wave propagation leads to formation of shocks, the scheme will detect a discontinuity present in the solution. The underlying physics of the upwind approach is based on a physical experiment called the Riemann problem. From Equation 2.1, the Riemann problem is defined as,

$$u(x,0) = \begin{cases} u_L, & x < 0 \\ u_R, & x > 0 \end{cases} \tag{2.2}$$

where u_L and u_R are constant.

At initial time, $t = 0$, the discontinuity is located at $x = 0$, when $u_L > u_R$, the solution forming shock wave, when $u_L < u_R$, rarefaction wave will be created due to the wave expansion and when $u_R = u_L$, the parallel waves move and be connected by a contact discontinuity. A Riemann problem assumes two fluid states (L, R) separated by a common interface. In order to solve Riemann problem, it requires solving the fluxes across each interface. The solution to the Riemann problem is based on the characteristics of the Jacobian matrix of the Euler conservation systems, thus the upwind scheme is called a characteristic based scheme. There are two approaches to solve the flux at the interface boundary, either exact (Godunov, 1959) or approximate [(Engquist and Osher, 1981), (Harten et al., 1983), (Roe, 1981), (Toro et al., 1994)]. Schemes that solve the Riemann problem is called Riemann solvers which is the basis of Flux Difference Splitting (FDS), one of the foundations of solving the FVM. Another approach in FVM and is known as the Flux Vector Splitting (FVS) method.

2.5.1 Flux Difference Splitting (FDS)

Exact Riemann solvers and approximate Riemann solvers are characteristic wave based approaches. The upwind directions are determined from the characteristic waves. The Exact Riemann solver was developed by Godunov, (Godunov, 1959). It is accomplished by solving Riemann exactly at each CV interface. Due to complexity and cost of the Exact solver problem, many researchers take other alternatives and developed approximate Riemann solvers. The approximate Riemann solvers discussed here are (1) the Osher flux, and (2) the Roe flux.

2.5.1.1 Approximate Riemann Solver

The Osher flux (Raimund et al., 2009) determines the direction of the flux by choosing the sign of the eigenvalues. The Osher flux was shown to be very accurate and particularly well suited for explicit upwind formulations. However, increasing accuracy will increase the computational cost and the complete linearization flux formula for implicit formulation becomes very complex. The main contribution to the computation cost is the determination of the intermediate states connecting the two states of the neighbouring grid points. Probably this is the reason why the Osher flux is not attractive to solve engineering problems with very complex hyperbolic systems.

The Roe flux (Roe, 1981) approximates the Jacobian matrix using an average of the state variables for left and right of the valuating cells. The Roe flux has minimal numerical dissipation, thus it produces the most accurate results compared with other approximate Riemann solvers. The Roe flux is popular and widely used for shock capturing scheme, because it is simple and very economical to setup (Roe, 1981). However, the Roe flux suffers from shock instability in strong shocks (Quirk, 1994) and low density flow which involves strong rarefaction waves. The Roe flux also suffers from capturing unphysical shock (expansion shock) but this can be remedied by entropy fix (Coirier and Powell, 1995).

2.5.2 Flux Vector Splitting (FVS)

For FVS, the numerical flux functions are computed by using the component technique. Unlike FDS, FVS ignores the interaction between the moving waves but rather splits the fluxes (F), into two parts: forward, (F^-) and backward, (F^+) components. The flux at the interface boundary is defined as

$$F_{i+\frac{1}{2}}(u_L, u_R) = F^+(u_L) + F^-(u_R) \tag{2.3}$$

The upwind direction is determined based on sign of the flux. There are two examples of flux function that uses FVS and they are; Steger-Warming Splitting (SWS) (Steger and Warming, 1981) and Van Leer Splitting (VLS) (Van Leer, 1982).

The SWS (Steger and Warming, 1981) introduced the flux splitting by using the sign of the wave speeds for inviscid Euler equations of gas dynamics. The flux is assigned (F^-) when the wave speed is negative sign, and (F^+) is set when the wave speed is positive sign. The SWS is attractive due to its simplicity because it does not worry about the direction of wave propagations and is suitable for implicit upwind scheme. Nevertheless, the downside of the SWS is that when there is a sonic point ($Ma = 1$), the flux produces some errors near the point because of the sign change of the wave speed.

The VLS (Van Leer, 1982) is an alternative to FVS which overcomes the SWS deficiency at the sonic point. The VLS is designed using special Mach number polynomials to construct fluxes so that the solutions remain smooth at sonic point and this refinement produces better results (Anderson et al., 1986). However, the VLS also produces poor resolutions due to excessive artificial diffusion like the SWS. The VLS and SWS fail to recognize the contact discontinuities and predict overly dissipated boundary layer. Significant errors are produced in the viscous region which cannot simply be cured by refining the grid size and/or using higher order differencing.

In short, the FVS approach is simple and efficient but its simplicity reduces the accuracy of the scheme mainly due to excessive numerical diffusion (Ren et al., 2003). This type of error is not associated with FDS because the Riemann solvers are able to recognize the contact discontinuity wave and predicts a much better boundary layer predictions.

2.5.3 Combinations of FDS and FVS

By taking the advantages of both FDS and FVS, a new method is developed by (Liou and Steffen, 1993) known as Advection Upstream Splitting Method (AUSM). In this method it does not involved any matrix operation thus makes it more efficient and easy to code. It has become a very popular numerical flux function.

The AUSM can converge as fast as the Roe solvers and the scheme is also remarkably simple and accurate. In addition, the AUSM scheme also is very efficient in the regions of very high pressure gradients like shock waves and discontinuities. However, the AUSM scheme also suffers from deficiencies which include the shock-instability problem (Kitamura et al., 2009).

2.6 High Resolution Upwind Differencing Schemes

Unfortunately, the first order results are too diffusive for continuous flow. Thus, second order or higher order accuracy schemes are needed to overcome the deficiencies. Higher order schemes also known as high resolution schemes have been designed to obtain higher order at continuous flow and then changed to first order when it is near the discontinuities to satisfy Godunov's Theorem [(Godunov, 1959), (Sweby, 1984)].

In order to design the high resolution scheme without producing oscillation at discontinuities, several guidelines need to be complied. Harten (Harten, 1983) had introduced Total Variation Diminishing (TVD) that implies Equation 2.5,

$$TV(u^{n+1}) = \sum_i \left| u_{i+1}^{n+1} - u_i^{n+1} \right| \tag{2.4}$$

$$TV(u^{n+1}) \leq TV(u^n) \tag{2.5}$$

where TV is total variation between variable values and u^n is the variable values at time level n. It means that, when summation of variation between the flow variables decreases with time, no spurious oscillations will be generated. As long as Equation 2.5 is satisfied, the spurious oscillations can be avoided. Numerical schemes that meet the TVD requirement are called TVD schemes.

2.6.1 Reconstruction Techniques

In order to obtain a higher order scheme, instead of taking constant piecewise state variables at the flux boundary, the variables at the CV centroid will be reconstructed to a linear function to obtain accurate values along the flux boundary. There are two types of reconstruction techniques: (1) MUSCL scheme, and (2) ENO and WENO scheme.

2.6.1.1 MUSCL Scheme

The Monotonic Upwind Scheme for Conservation Laws (MUSCL) developed by Van Leer (Van Leer, 1979) is widely used for higher order TVD schemes. It uses a linear reconstruction to process the Riemann solutions to achieve second order accuracy (or higher). However, the slope of piecewise linear distribution is limited, to avoid spurious oscillations around a discontinuity.

2.6.1.2 ENO and WENO Scheme

(Harten and Osher, 1987) developed the Essentially Non-Oscillatory (ENO) scheme which allows the loss of amplitude at one time step to be gained at another for the sake of achieving very high order accuracy. Later, (Liu et al., 1994) proposed the Weighted Essentially Non-Oscillatory (WENO) scheme for improvement. For high order spatial discretizations, a WENO reconstruction technique provides the reconstruction polynomials in terms of a hierarchical orthogonal polynomial basis over a reference element (Dumbser et al., 2007).

Both schemes have demonstrated very promising shock capturing capabilities. Because they achieve the user defined high order accuracy while avoiding spurious oscillations, these schemes have been widely used for shock capturing. However, drawbacks still exist with these schemes since small amplitude waves might be damped and the fact that it does not include any precise entropy control.

2.6.2 Flux Limiters

The steep gradient near the discontinuity will produce spurious oscillation around discontinuities with the absent of limiters. The flux limiter ensure that the scheme complies with the TVD principles in Equation 2.5. In order to prevent the occurrence of artificial oscillations in the high resolution scheme, the flux limiters will enforce a constraint to the gradient of the flux function. The constraint will determine either to use high order for smooth regions or first order for discontinuous regions or somewhere in between.

The Flux-Corrected Transport (FCT) scheme is a flux limiter developed by Boris and Book (Boris and Book, 1973). The FCT is a high order at the smooth regions. For the discontinuities, the FCT adds the right amount of dissipation near shocks. There are two additional steps in this scheme to optimize the shock quality. First, it will add anti-diffusive flux where the solutions are stable but diffusive to remove excess dissipations. Then, the flux limiter is applied to the solutions to ensure that no oscillations occur. This approach is the same with TVD in principle; that is to make sure monotone solutions are obtained for discontinuous problems; yet maintaining high order accuracy when the flow is smooth. The FCT is very robust but the FCT produces over dissipation in open channel test problem (Yost and Rao, 1999). This is due to the excessive artificial diffusion in smooth regions with large gradient.

2.6.3 Slope Limiters

After values at flux boundary has been reconstructed by the neighbouring cells, slope limiters are used to control unnecessary oscillations in the solutions. The ratio of left and right gradient, r will be the function for slope limiters, and choosing the nonlinear average in such a way that the total variation of the reconstructed function is no greater than that of the underlying cell averages.

The slope limiters discussed herein includes Superbee (Roe, 1985), Van Leer (Van Leer, 1974) and minmod limiters. The Minmod limiter is the minimal second order for TVD scheme. Thus, it is the most diffusive limiter because it takes the minimum between slope right and left. Although, minmod limiter tends to produce not very accurate results but it is most stable limiter. Moreover, it can guarantee there is no oscillation present in the solutions. Minmod limiter has always been chosen as the benchmark comparison with other complex limiters due to its simplicity and robustness.

The Van Leer limiter (Van Leer, 1974) is a smooth curve lying between Minmod limiter and Superbee limiter. It has a smooth region that is a monotonically increasing function satisfying the symmetry property. It is not as diffusive like Minmod limiter and is minimally dissipative almost as good as Superbee limiter. It is in between the stability of Minmod limiter and the accuracy of Superbee limiter. The Van Leer is a reliable limiter and satisfies the TVD constraint.

The Superbee limiter of Roe (Roe, 1985) is known as the most accurate and least diffusive limiter. The Superbee limiter also provides an anti-diffusion mechanism, steeping the flow profile when there is no danger of overshooting thus increasing the accuracy.

2.7 Second Law of Thermodynamics

The first law of thermodynamics states that energy is conserved. Energy can neither be created nor destroyed. The first law of thermodynamics is one of the fundamental concepts of physics along with conservation of mass and conservation of momentum. The second law of thermodynamics states that "if no energy enters or leaves the system, the potential energy of the state will always be less than that of the initial state". In other words, the system will always move to be more chaotic. This is also commonly referred to as the nature of entropy generation. The Roe flux does not precisely adhere to the second law of thermodynamics which governs the laws of entropy generation. Strictly speaking, entropy should not be produced for continuous flow. Yet most, if not all numerical schemes in CFD will generate spurious (artificial) entropy. Usually a test of a good CFD method is that it produces the minimum entropy for continuous flows and this is rarely met even for simple flows. On the other hand, a discontinuous flow such as flow across a shock, entropy should be produced not only with the proper sign but also in proper amount.

2.8 Numerical Schemes for Entropy Stability

A system of conservation laws with entropy generation is essential in satisfying the second law of thermodynamics for numerical schemes. In order to design the numerical schemes which comply to the thermodynamics's law, (Harten, 1983) derived entropy pairs for systems of conservation laws exclusively for NS equations neglecting heat conduction. This study has been the crucial point in development of entropy stable conservative schemes which has been referred to by later researchers. As an example, the symmetrization of conservation laws of gas dynamics derived by (Harten, 1983), initiated (Hughes et al., 1986) to develop finite element methods where the entropy is conserved. Also, the entropy pairs (Harten, 1983) was an initial point for (Tadmor, 1986a) to derive minimum entropy principle for the conservative Euler equations. The research on the system of entropy stable conservative scheme has developed into several techniques which are, (1) numerical viscosity, (2) physical viscosity, (3) combination of numerical and physical viscosity, (4) kinetic relations, and (5) TeCNO scheme.

2.8.1 Numerical Viscosity

The concepts of entropy and viscosity are related to each other for systems of conservation laws. The artificial dissipation which is mostly viscosity term can suppress spurious oscillation across shocks due to improper treatment of entropy at the shocks. In year 1984, (Tadmor, 1984) had added numerical viscosity into the conservation laws system and compared it with other entropy conservative schemes. (Tadmor, 1984) concluded that the new scheme is stable when it has more numerical viscosity. Later in 1987, (Tadmor, 1987) quantified the additional amount of numerical viscosity in the Euler conservative scheme to acquire entropy stability.

The second order entropy conservative flux was introduced in (Tadmor, 1986b) and (Tadmor, 1987) by using finite element discretization. The schemes are proven to be entropy consistent and lot of researchers use the technique as a reference [E.g. (Hayes and LeFloch, 1998), (Chalons and LeFloch, 2001b), (Fjordholm et al., 2008) and etc.]. Unfortunately, the down-side of the scheme is that the equations are complex to code and that the amount of numerical viscosity being used is not based on precise science.

2.8.2 Physical Viscosity

The new family of the second order difference schemes by (Tadmor and Zhong, 2006) and (Tadmor and Zhong, 2008) using physical dissipation terms instead of artificial numerical scheme (Tadmor, 2003) as entropy dissipation. The physical dissipations which are viscosity and heat conduction are on right hand side (RHS) of the NS conservation equation. This full NS equations with viscosity and heat fluxes are fully explicit third-order Runge-Kutta (RK3) time integration. The schemes have a flexibility for every system of entropy conservative schemes.

Nevertheless, the computational cost for this scheme is very expensive and it requires a very fine mesh to produce smooth results (Tadmor and Zhong, 2006), (Tadmor and Zhong, 2008). For the 1D Sod's tube test problem, the Tadmor & Zhong method uses a grid of 1000 mesh where $\Delta x = 0.001$, compared with other schemes which use ten times coarser mesh yet the other schemes still produced better results [(Fjordholm et al., 2012a), (Ismail and Roe, 2009)]. This is not an efficient scheme to solve 2D or 3D engineering problems when the grid size becomes crucial factor in designing a new scheme.

2.8.3 Combination of Numerical and Physical Viscosity

The idea to include physical viscosity from (Mohammed and Ismail, 2013) is a continuation of entropy consistent Euler flux from (Ismail and Roe, 2009). The entropy consistent Euler flux was designed to solve inviscid flow and depends only on the artificial diffusion. This work takes (Tadmor and Zhong, 2006) as a reference for comparison since Tadmor and Zhong applied fully physical dissipation in their scheme. (Mohammed and Ismail, 2013) had incorporated physical viscosity into the inviscid flux of (Ismail and Roe, 2009) to solve NS equations with no heat transfer. To achieve entropy consistency for the new method, the approach was to include physical and numerical viscosity as mechanisms to generate entropy. The tests had run from low viscosity to high viscosity conditions for several cases. This method which is not relying solely on physical viscosity shows that it is not too expensive as (Tadmor and Zhong, 2006) but produce good results. Nevertheless, this preliminary study is still in the process of development. In addition, the results therein only focus on laminar flow where the physical viscosity is constant.

2.8.4 Kinetic Relations

(Fjordholm et al., 2002) had designed entropy conservative fully discrete schemes with high order accurate entropy conservative flux. The scheme includes discretization of the diffusive and dispersive terms of the continuous model. (Chalons and LeFloch, 2001b) was the first to initiate fully discrete schemes for diffusive dispersive conservation laws. The schemes added by selecting a mechanism called kinetic relation to make entropy equality to have a unique solution for the system. By comparing discrete and continuous models, the kinetic functions have been calculated to provide entropy dissipations across a shock. Several works on the kinetic relations such as (Hayes and LeFloch, 1997), (Hayes and LeFloch, 1998), (Hayes and LeFloch, 2000), (LeFloch and Rohde, 2000), (Chalons and LeFloch, 2001a) are very important.

The schemes are specifically designed to study the system of conservation laws and to determine whether the schemes have nonconvex modes or a hyperbolic-elliptic system. Consequently, the schemes are only limited to solve weak and moderate shocks. When the scheme experiences strong shocks, the results produce instabilities due to some limitation. This is because the kinetics of continuous model cannot be reproduced using numerical methods for strong shocks. However, before the work of (Roe, 2006) most of this entropy schemes are strictly academic since they are implicit and complicated to be used in engineering problems.

2.8.5 TeCNO scheme

(Fjordholm et al., 2012a) emphasized on the construction procedure of high order accurate entropy stable semi discrete scheme named TeCNO scheme. The TeCNO scheme focuses on reconstruction of higher order scheme while using explicit diffusion operator from (Ismail and Roe, 2009). Basically, the scheme is based in two parts, (i) entropy conservative flux, using procedure of (Fjordholm et al., 2002) to obtain higher order accurate entropy conservative flux, and (ii) numerical diffusion operator, using new explicit solution for the Euler equation designed by (Ismail and Roe, 2009). Continuation from 1D test problem (Fjordholm et al., 2010), (Fjordholm et al., 2012a) had tested the scheme for 2D test problems.

In order to construct entropy conservative schemes, (Fjordholm et al., 2012a) followed a different approach from (Fjordholm et al., 2008) because of it deficiencies. (Fjordholm et al., 2008) had designed energy preserving and energy stable schemes particularly for shallow water equations. The schemes are numerically unstable and produced high oscillations near shocks. Therefore, Fjordholm et. al necessarily introduced some dissipative mechanism into the scheme to ensure that entropy dissipated across shocks (Fjordholm et al., 2010),(Fjordholm et al., 2012a). (Fjordholm et al., 2012a) constructed high order numerical diffusion operator (Roe-type) by using modified ENO reconstruction procedure of the entropy variables to ensure entropy stability (Fjordholm et al., 2011).

Fjordholm et. al agreed with (Ismail and Roe, 2009) that the explicit solution is computationally inexpensive for entropy conservation fluxes system. TeCNO schemes are weakly converge to constant-coefficient symmetrization system. However, this method cannot converge to scalar nonlinear conservation laws of high order. In addition to this, TeCNO scheme is limited to structured grid on account of its finite difference scheme.

2.9 A New Entropy Consistent Euler Flux

This is a new capturing method developed by (Roe, 2006) and (Ismail and Roe, 2009) in an attempt to overcome deficiencies of the Roe flux when dealing with shock instability. The new flux function is named Entropy Consistent Euler flux