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Development and Assessment of Upwind Schemes with Application to Inviscid and Viscous Flows on Structured Meshes

by

Mohammad Jafar Kermani

A thesis submitted to
the Faculty of Graduate Studies and Research
in partial fulfillment of
the requirements for the degree of
Doctor of Philosophy

Ottawa-Carleton Institute for
Mechanical & Aerospace Engineering

Department of
Mechanical & Aerospace Engineering
Carleton University
Ottawa, Ontario
June, 2001

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Meshes**

Submitted by

Mohammad Jafar Kermani

In partial fulfillment of the requirement for the degree of
Doctor of Philosophy of Engineering

A handwritten signature in cursive script, appearing to read "Robert Bell", written over a horizontal dashed line.

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June 25, 2001

Abstract

Two major categories of Upwind Differencing (UD) algorithms, namely flux vector splitting and flux difference splitting are studied and modified during the course of this research. These schemes are the van Leer scheme from the FVS family and the Roe scheme of the FDS type. To check and assess the accuracy of the modified algorithms the inviscid Burgers equations, Riemann problem (shock tube problem) and Euler equations in two-dimensions are taken as model equations. The method is later extended to the Navier-Stokes equations.

For the spatial discretization of inviscid terms (convective and pressure terms) three different cases are studied: (1) second order upwind scheme, in which the numerical oscillations are damped by minmod Total Variation Diminishing (TVD), (2) third order upwind biased scheme with the van Albada flux limiter and (3) mixed second and third order scheme with no flux limiter. In cases (1) and (2) the primitive variables are extrapolated to the left and right faces of the cell by the Monotone Upstream-centered Schemes for Conservation Laws (MUSCL) idea, while in case (3) the inviscid fluxes are directly extrapolated to the cell faces. For the spatial discretization of the viscous terms, central difference is used. For the temporal discretization, either Euler's first order forward, or second order two step predictor-corrector from the Lax-Wendroff family is used. The governing equations are recast into generalized coordinates and are solved in these coordinates.

The method is applied to a variety of test cases ranging from the low subsonic regime (Mach of 0.5) to supersonic flows (Mach 4.0). Turbulence is modeled by the Baldwin and Lomax zero-equation model. The meshes, which are structured, are developed by an algebraic or by an orthogonal grid generator in a separate module and then transferred to the main solver.

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Dedication

to my mother & my wife who suffered the most during my studies.

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Chapter 1

Introduction

1.1 Motivations

Experimental results have always been extremely valuable in validating mathematical solutions of the governing equations of fluid motion (Hoffmann and Chiang (1993)). On the other hand daily growth in the capability of computer hardware constantly increases the interest in using Computational Fluid Dynamics (CFD) as a tool to solve, analyze, design and/or investigate the challenging and complex problems of fluid dynamics and heat transfer. One example is cited to elaborate on this issue explaining our now vital need to use CFD as a complementary tool of designing and analyzing problems containing fluid flows with heat exchanges.

In late 1970's, this approach (the use of supercomputers to solve aerodynamic problems) began to pay off. One early success was NASA's experimental aircraft called HiMAT. Wind tunnel tests of a preliminary design for HiMAT showed that it would have unacceptable drag at sonic speeds and the model-plane would be unable to provide any useful data. The cost of redesigning it for further wind tunnel tests would have been around \$150,000 and would have unacceptably delayed the project. Instead, the wing was redesigned by a computer at a cost of \$6,000 (Anderson (1995)).

This example shows how CFD is now an inseparable organ of the body of design (or analysis) of today's fluid problems and it will be so for the foreseeable future.

However, the need to make CFD a precise tool of study and research is a hard and time demanding task because after the numerical schemes are designed they have to pass a certain number of determining tests. In addition, they have to be robust and universal. So improvement of any numerical algorithm in any degree, even a small improvement, becomes a very challenging but an interesting task; especially as the algorithms have significantly become mature and mature by the inputs from scholars in this field over many years.

The accuracy improvement of numerical algorithms is now the major and core part of the CFD research, the matter which has been under constant development and improvement since their inception. The objective is to make CFD an accurate tool to precisely capture and detail the physics of the flow as much as it is possible. This requires special attention to be given to many details when a numerical algorithm is being designed.

The science of CFD goes back many years, but the 1970's can be considered as the development period for the foundation of central discretization algorithms for the Euler and Navier-Stokes equations (Hirsch (1990)). The physically based algorithms (upwind schemes), which have their roots in Godunov's method, were the focus of CFD researchers in the 1980's. To further improve the accuracy, robustness and efficiency of numerical algorithms, there continue to be challenges of interest to CFD researchers.

1.2 Objectives

In brief, the objectives of this thesis could be listed as:

1. to modify selected existing upwind algorithms in order to enhance their accuracy, robustness and efficiency in solving the fluid equations,
2. to examine and to assess the capability of the modifications, by developing a CFD code to demonstrate their use, and
3. to provide a code which will eventually apply the method to aerospace applications.

1.3 Structure

To achieve the objectives of this thesis, a sequence of steps has been carried out. The sequence is:

(I) Step I, in which two-dimensional viscous flow was simulated, based on the MacCormack explicit predictor-corrector scheme (1969). It was basically planned to prepare the author of the thesis to use advanced and smart numerical schemes. This step, which could be called as the homework step, was applied to laminar supersonic flow including flow between two plates. Shock-shock interaction and shock interaction with boundary layers are observed in this step (see Kermani and Plett (1996)).

(II) In step II, the van Leer scheme (1982) is taken as the model upwind scheme and a non-oscillatory numerical algorithm has been developed by blending appropriate weighting from the second- and third-order flux derivatives without any limiter. Basically in this part of the thesis, it is verified that the standard second-order scheme is unable to give a non-oscillatory solution without a flux limiter. This is even worse when the standard third-order scheme is applied without limiter. However, when appropriate weighting from the second- and third-order definitions of the flux derivatives are blended, the oscillatory diverging terms of the second and third order terms cancel each other and a non-oscillatory scheme is obtained in the absence of any flux limiter. The weighing factor (blending factor) of the second- and third-order accurate derivatives obtained in this study are: $W_{2nd} = 7/4$ and $W_{3rd} = -3/4$, which have been used for all the test cases performed. This algorithm has been applied to fluid flows containing sharp gradients and agreement with analytical results has been with less than 4% of error. The results of this study for two-dimensional planar test cases are given in the paper by Kermani and Plett (1998^a). With the same blending factors, the method has later been extended to two-dimensional axi-symmetric flows (see Kermani and Plett (1998^b)) and very accurate results were obtained.

(III) Step III, introduces a simple modification to the Harten entropy correction formula, as applied to Roe's FDS scheme (1981). This modification basically en-

larges the band over which the Harten entropy fix condition is enforced by a factor of four. The resulting formulation, as opposed to its ancestor, is able to totally remove the non-physical expansion shocks from the sonic expansion regions without impressing the rest of the computational domain (see Kermani and Plett (2001^a)).

(IV) Step IV, in which a new and simple approach has been adopted to obtain the numerical flux for the Roe scheme based on the flow parameters and the grid-geometry in generalized coordinates. The primitive variables are extrapolated to the cell faces by the MUSCL idea using the third order upwind biased scheme. Two flux limiters (or TVD), namely, minmod (see for example Tannehill et. al. (1997) and van Albada (1982)), are used to prevent spurious numerical oscillations (see Kermani and Plett (2001^b) and (2001^c)).

Roe's FDS scheme with the implemented modifications as given in III and IV has been extended to viscous flows governed by the Navier-Stokes equations, in which central differencing is used for the discretization of diffusion terms as usually recommended in the literature. For the turbulent flow computations, a simple eddy viscosity model (Baldwin-Lomax (1978) model) is used.

1.4 Outline

This thesis contains seven chapters and five appendices. The following strategy is applied when writing this thesis. The first and the last chapters of this thesis are the introduction and conclusion to the thesis, respectively and Chapter 2 is devoted to review of the previous work. The central body of the thesis, Chapters 3, 4, 5 and 6, are the materials covered, obtained, or derived throughout this thesis research, which could be a considered a detailed explanation of the contributions made by this thesis.

The materials included in Appendices A to D may be found in the literature with some minor differences (see for example Hoffmann and Chiang (1993), Tannehill et. al. (1997) and/or Hirsch (1990)). However, because these materials were in close relations with the course of this research, they are included in this thesis. On the other hand, the materials of the appendices have intentionally been kept away from

the core part of this thesis in order to make the body of the thesis, i.e. Chapters 3 to 6, focused on the work performed merely for this thesis. In detail the outline of this thesis is:

1. Chapter 1, the current chapter, gives an introduction to the thesis.
2. Chapter 2 reviews the literature related to the work performed, which resulted in this thesis.
3. Chapter 3 is totally allocated to the development and assessment of the upwind numerical algorithm as applied to the van Leer scheme by blending the second and third order accurate derivatives of convective fluxes- see step II in Section 1.3.
4. Chapter 4 covers the entropy correction formula as applied to the Roe scheme and its accuracy assessment, which is outlined in step III of Section 1.3.
5. Chapter 5 explains how the numerical flux for the Roe scheme is obtained in generalized coordinates - step IV in Section 1.3.
6. Chapter 6 is the application (to inviscid and viscous flows) of the formulae obtained for entropy correction and numerical flux as given in Chapters 4 and 5, respectively.
7. Chapter 7, final chapter, includes the concluding remarks, list of contributions and suggestions for future works.

The appendices included in this thesis, basically explain the fundamentals of upwinding as applied to the wave equation and the Riemann problem (shock tube problem).

1. Appendix A explains the physical and numerical solutions of the wave equation and how the fundamental equations of the flux vector splitting (FVS) and the flux-difference splitting (FDS) schemes are obtained by applying them to the wave equation.

2. Appendix B explains the decomposition of fluid equations, in which a form similar to the wave equation is obtained.
3. Appendix C describes the solution of fluid equations by FVS and FDS schemes.
4. Appendix D brings together a complete formulation of the Roe scheme in a single place, i.e. in a single appendix, for one- and two-dimensions.
5. Appendix E lists the publications related to this thesis.

Chapter 2

Review of Previous Work

2.1 Introduction

The current chapter of this thesis is intended to review the previous work in the numerical schemes available for CFD. However, it is not intended to give a catalog, handbook, or even a list of the numerical techniques available in the literature. The chapter begins with a broad classification of the numerical schemes found in the literature. Then an attempt is made to obtain an appropriate category, which meets the objectives of the thesis, as outlined in Section 1.4. This is done because, the type of the numerical schemes are quite versatile and each cannot be discussed in comprehensive detail. Moreover, to do so would be beyond the scope of the current study. However, attempts will be made to shorten the list by eliminating those schemes which are considered as not appropriate for the current study.

This will allow the list to be shortened as quickly as possible and to reach the desired numerical scheme, which will be adopted in the current study, and to spend more critical review on the selected schemes.

The selected schemes, for which critical study will be performed, are two major categories of upwind schemes, namely the Flux Vector Splitting (FVS) and Flux Difference Splitting (FDS) schemes. Moreover, to keep this chapter a formulae-free chapter as much as possible, the development of the formulae of these two categories of upwind schemes are included in four appendices at the end of this thesis, rather

than in this chapter.

2.2 Classification of Numerical Schemes; A Broad View

Numerical schemes can be broadly classified into various groups. They could be grouped as follows: (1) pressure-based schemes as compared to density-based schemes, (2) central differencing schemes as compared to upwind schemes, (3) shock-capturing schemes as compared to shock-fitting schemes, and (4) steady flow computation, with unsteady equations. To clearly describe the differences between the shock capturing and shock fitting schemes, a model equation, namely, one-dimensional inviscid fluid equation is first introduced then the idea of shock capturing vs. shock-fitting is given. Some types of time and space discretization are also reviewed and discussed in this chapter.

2.2.1 Pressure-Based vs. Density-Based Techniques

Based on the Mach number of a flow, one can roughly divide the flow into several regimes, namely, incompressible ($\text{Mach No.} = 0$), subsonic/constant density ($0.0 < \text{Mach No.} < 0.3$), subsonic/variable density ($0.3 < \text{Mach No.} < 0.6$), transonic ($0.6 < \text{Mach No.} < 1.2$), supersonic ($1.2 < \text{Mach No.} < 6.0$), hypersonic ($6.0 < \text{Mach No.} < 25.0$). This is because each regime is characterized by different phenomena. For example, in the transonic regime, shocks can only appear in the supersonic portion of the flow. On the other hand, in supersonic flow, shocks can be the dominant feature. At the hypersonic flow end, there will be strong shock/boundary layer interactions, and real gas effects. In order to obtain accurate solutions, one must take into account these unique features for each flow regime. In this section the classical pressure-based and density-based approaches are described and the shortcoming of each is briefly explained. This is followed by a recent approach which uses the advantages of both.

The classical pressure-based algorithms, or pressure-correction methods, start the solutions by solving the momentum equations with some guessed values for the

pressure field. The resolved velocity components are then placed into the continuity equation and an equation for the pressure correction, an elliptic equation (like the Poisson equation) is obtained and then solved to give the magnitude of the pressure correction. Pressure is updated by adding the old value to the pressure correction and the procedure is repeated until the computed velocity domain satisfies the continuity equation (i.e. the magnitude of the pressure correction sufficiently reduces as the solution advances). One of the most commonly used methods of this family is due to Patankar (1980). This method was originally developed for incompressible flows (Mach No.=0.0), and later extended to compressible flows. However, schemes based on classical pressure-based methods are more appropriate for incompressible flows and the low speed regimes than the high speed flows. In high speed application, these schemes have a major shortcoming, which is in the form that the governing equations are written. That is the governing equations are not written in the full conservative form. For example, pressure gradients are not written as part of inviscid fluxes by combining with convective terms. Therefore, in the vicinity of large gradients like shock waves, where the primitive variables undergo large changes, these types of schemes show a non-satisfactory behavior leading to oscillatory solutions and shock smearing.

A density-based method, which includes the density as one of the primitive variable, has been firstly designed for compressible flow. However, the extension of these methods to flows with low Mach number has also been possible by correction for incompressibility effects. Some of the most widely used density-based methods are those by MacCormack (1969), Jameson (1981), van Leer (1982) and Roe (1981).

Density-based schemes at low Mach numbers become numerically stiff as density becomes almost an invariant primitive variable and results in poor convergence rates. This becomes a severe problem for incompressible flows in which acoustic waves travel with infinite speed theoretically. This difficulty has been resolved by employing pressure as one of the primitive variables instead of density and by a preconditioning matrix applied to the time derivative term of the governing equations (unsteady term of the governing equations), see Fiterman et. al. (1995) for example. The preconditioning re-scales the acoustic speeds (or the eigenvalues of

the Jacobian matrix) and significantly reduces the stiffness of the governing equations in low speed regimes. The inclusion of the preconditioning matrix to re-scale the acoustic speeds introduces extra complexity to the flow solver. For the current study, in which the flow regimes of Mach number =0.5 and greater are studied, density-based schemes are chosen.

2.2.2 Central vs. Upwind Differencing Schemes

Consider the fluid equations in full conservation form written in Cartesian coordinates:

$$\frac{\partial Q}{\partial t} + \underbrace{\frac{\partial F_{inv}}{\partial x} + \frac{\partial G_{inv}}{\partial y}}_{\text{inviscid terms}} = \underbrace{\left(\frac{\partial F_{vis}}{\partial x} + \frac{\partial G_{vis}}{\partial y} \right)}_{\text{viscous terms}}, \quad (2.1)$$

where Q is the conservative vector, F_{inv} and G_{inv} are the inviscid fluxes and F_{vis} and G_{vis} are the viscous fluxes. Numerical schemes to solve Eqn. 2.1 can be broadly classified as central or upwind differencing schemes, based on the spatial discretization of inviscid terms in Eqn. 2.1. It is noted that viscous terms in Eqn. 2.1 are always discretized by central differencing, regardless whether the inviscid terms are discretized by central or upwind schemes. The idea of spatial discretization of inviscid terms by central or upwind schemes is discussed in this section.

Consider the inviscid term $\partial F_{inv}/\partial x$, which is approximated in node j by: (see Fig. 2.1)

$$\left(\frac{\partial F_{inv}}{\partial x} \right)_j \approx \frac{F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}}}{\Delta x} \quad (2.2)$$

where $F_{j+\frac{1}{2}}$ and $F_{j-\frac{1}{2}}$ are the numerical fluxes at the East (E) and West (W) boundaries of the cell j , respectively, as shown in Fig 2.1. Numerical fluxes $F_{j+\frac{1}{2}}$ and $F_{j-\frac{1}{2}}$ are denoted in short by F_E and F_W for convenience. Therefore:

$$\left(\frac{\partial F_{inv}}{\partial x} \right)_j \approx \frac{F_E - F_W}{\Delta x}. \quad (2.3)$$

In Eqn. 2.3, the numerical fluxes F_E and F_W are determined from the flow parameters and grid geometry in neighboring nodes. The type of the formulae for the numerical fluxes F_E and F_W determines the numerical scheme by which the computation is performed. For example, the numerical flux F_E based on central difference

scheme is given below. Once F_E and F_W are determined based on the type of numerical scheme, they are substituted into Eqn. 2.3 to give the gradients of inviscid flux.

The most obvious choice to obtain the numerical flux at the cell face is the central difference (CD) scheme, in which F_E is determined from:

$$F_E = \frac{1}{2} [F_j + F_{j+1}]. \quad (2.4)$$

As shown in Eqn. 2.4, CD discretization is based on a symmetric choice of the information stored in the neighboring nodes of the cell face, see Fig. 2.1. That is CD schemes do not take into account the side from which information arrives at the cell face, and they ignore the typical essence of hyperbolic problems, in which information is propagated along specific lines, called *characteristic directions*. They treat both upstream and downstream of the cell face in the same manner (as may be appropriate in a diffusion problem).

Moreover, CD schemes are not robust (a computer code is described as being *robust* if it has the potential of giving reliable answers to a wide range of problems without needing to be re-tuned). In this regard, CD schemes usually require one adjustable parameter to be tuned to control the amount of numerical dissipation and usually another one to stabilize, or to smooth the solution against checkerboard oscillations. The magnitude of these parameters are usually case dependent and are unknown prior to each test case and should be optimized depending on the type of problem. The popularity of CD is mainly attributed to the ease with which such algorithms can be implemented. Some of the popular CD schemes are those developed by Beam and Warming (1978), MacCormack (1982) and Jameson (1981).

As opposed to diffusion problems in which a symmetric contribution from upstream and downstream are desired, upwind differencing (UD) schemes are designed on the basis that information propagates along the characteristic direction in the physical domain. Therefore, these types of schemes are in good agreement with the physics of the flow of information throughout the fluid flow field. Also these schemes are robust as they are naturally diffusive. However, on the other hand, UD schemes are much more complicated to code and extra memory space is needed to obtain the

acoustic wave speeds, (eigenvalues), which determine the direction from which the information arrives at the point of interest.

Two major categories of UD schemes, namely flux vector splitting and flux difference splitting schemes, are explained later in detail in this chapter.

2.2.3 Model Equation

To better explain the idea of shock capturing schemes versus shock fitting techniques, as given in the next section, a model equation is developed first. This equation is the governing equation of the fluid motion for one-dimensional inviscid flow of a compressible gas in a constant area duct, which obeys the following equations for conservation of mass, momentum and energy in the full conservation form (see Anderson (1995)):

$$\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} = 0 \quad (2.5)$$

where:

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho e_t \end{bmatrix}, \quad F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (\rho e_t + p)u \end{bmatrix},$$

t is time, x distance, ρ density, u velocity, p pressure, and e_t specific total energy. The system is closed by an equation of state $p = p(\rho, e)$, where e is the specific internal energy, $e = e_t - \frac{1}{2}u^2$. For a perfect ideal gas whose ratio of specific heats, γ , is constant, we have:

$$p = \rho(\gamma - 1)e \quad (2.6)$$

2.2.4 Shock Capturing vs. shock Fitting Schemes

The governing equation of fluid motion as given by Eqn. 2.5, is intentionally written in full conservation form. That is, the derivatives of the primitive variables of the flow, i.e., p , ρ , and u do not explicitly appear in the governing equation. However, the components of the flux vector F like ρu , $\rho u^2 + p$, and $(\rho e_t + p)u$ (see Eqn. 2.5), undergo a continuous process across the discontinuities as shown in Fig. 2.2. Therefore,

the numerical scheme leads to a better performance in terms of stability in capturing flow discontinuities like shock waves (more details could be found in Anderson (1995) or Kermani and Plett (1996)). This approach is suitable for the so called *shock capturing* approach, where discontinuities naturally appear in the domain of computation as a part of the solution.

Another method used to solve the fluid equations is based on the equations that are written in the so called *non-conservative* form, in which the governing equations are written in terms of primitive variables p , ρ , and u . This leads to an unsatisfactory behavior of the numerical solutions in the vicinity of discontinuities, as the primitive variables undergo large changes across discontinuities. This approach is usually applied to problems in which no sharp gradients are experienced within the domain of computations and could be studied by the so called *shock fitting* techniques. In shock fitting techniques, the use of strong or weak formulations of the equations do not affect the solution. In fact, in the shock fitting techniques, the domain of computation is split into the number of separated sub-domains each being a shock free domain, where these sub-domains are linked to each other by Rankine-Hugoniot relations.

A major shortcoming of the shock fitting approach is that a good knowledge of shock position is needed prior to the computation, which usually requires a cumbersome iterative approach for the trial and error to guess the shock locations. For this reason, the shock fitting techniques are almost always replaced by shock capturing in the recent literature. For the course of this study, the governing equations used are in the full conservative form and the technique used to solve the fluid equations is shock capturing.

A variety of shock capturing techniques are addressed in the literature. Some of the most important ones are: (1) Essentially non-oscillatory (ENO) schemes (see Laney (1998) for example), Total Variation Diminishing (TVD) (see Tannehill et. al (1997) and Hirsch (1990) for example) and compact TVD (see Tenaud et. al. (2000) for example). A comparison and review of these shock capturing techniques are performed by Tenaud et. al. (2000), in which the level of dispersion and diffusion of each of the shock capturing techniques are examined. They have concluded that

ENO schemes give the most accurate results for the test cases they have performed. However, ENO schemes are very complex to code in order to bring the numerical oscillations under control (see Laney (1998)), therefore, they are usually not used and it is preferred to employ a high resolution numerical scheme with a flux limiter.

2.2.5 Steady Flow Computations; Why Unsteady Equations?

For steady flow computations containing shock waves the fluid equations are usually taken in unsteady form. This results in one extra independent variable by extending the complexity of the governing equations in another dimension. Why is this approach preferred? The answer to this question is briefly given in this section. More detail in this regard could be found in Anderson (1995) or Kermani and Plett (1996)).

Consider a mixed supersonic-subsonic flow. The governing equations of the fluid motion are hyperbolic in the supersonic region; while they are elliptic in the subsonic region. The numerical solution techniques required in each of these regions are quite different. If the location of the shock waves are known, then in each region the appropriate solution could be sought according to the shock fitting technique, as mentioned in Section 2.2.4, and a time-independent type of fluid equation could be taken in each region. However, this problem is much more difficult to solve when the location of shocks are unknown, therefore, the problem is then solved as follows.

By introducing another independent variable, time, the governing equations become hyperbolic in time for the whole domain, regardless of whether the flow is locally supersonic or subsonic. This allows the mixed supersonic-subsonic flow to be treated in a unified manner. In this approach, a single technique is utilized to solve the entire flow field (previously governed by hyperbolic and elliptic equations), which is governed now by hyperbolic PDE's in time for the whole flow field.

In this approach the governing equations become hyperbolic only in time, i.e., the solution at the later time is dependent on the solution in earlier time. In this approach the steady state solution is obtained by marching the solution in time. This strategy is one of the most sophisticated techniques for the solution of all the

compressible flow solvers. Most importantly, for the time-dependent problems, the prescribed method could be used by taking appropriate time steps and a physically correct initial condition.

2.3 Time Integration

Time discretization (or time integration) techniques of the fluid equations are explained in this section. Basically the matter of time discretization describes to how to approximate the time dependent term $\frac{\partial Q}{\partial t}$ as given in Eqn. 2.5.

The simplest way of performing time integration is the explicit first order forward difference in time as referred to by forward Euler (see Tannehill et. al. (1997)):

$$Q^{n+1} = Q^n + \Delta t \left(\frac{\partial Q}{\partial t} \right)^n \quad (2.7)$$

where $\left(\frac{\partial Q}{\partial t} \right)^n$ is replaced by $-\left(\frac{\partial F}{\partial x} \right)^n$ from Eqn. 2.5. If the solution is linear in time, $\left(\frac{\partial Q}{\partial t} \right)$ is time-invariant, the time step Δt can be taken as large as needed and accurate results can still be obtained. But if the time rate of change is non-linear, which is usually the case, $\left(\frac{\partial Q}{\partial t} \right)$ varies along a curve and the solution of Eqn. 2.5 by Eqn. 2.7 will always have some errors. This error in the numerical integration can be magnified or accumulated in the path of time integration and at some point in time it can prevent further time integration because of the poor quality of integrated solutions. Therefore, the time step for the integration must be carefully chosen in order to avoid the accumulation of errors in the numerical integration. According to Hoffmann and Chiang (1993), a numerical scheme is said to be stable if any error introduced in the time integration does not grow with the solution. Δt in Eqn. 2.7 cannot be chosen arbitrarily but is limited by the stability criteria of the numerical solution. The size of time-step taken for each cell is limited by the least time taken by any of the acoustic waves to transverse the extent of the computational cell. For example three time steps for Eqn. 2.5 could be found, each giving the time step determined from the corresponding acoustic wave speed:

$$\Delta t_1 = \left| \frac{\Delta x}{\lambda_1} \right|, \quad \Delta t_2 = \left| \frac{\Delta x}{\lambda_2} \right|, \quad \Delta t_3 = \left| \frac{\Delta x}{\lambda_3} \right| \quad (2.8)$$

where $\lambda_1 = u - c$, $\lambda_2 = u$ and $\lambda_3 = u + c$ are the acoustic wave speeds and c is the speed of sound (for more detail, the reader is referred to Appendix B) and the smallest time step is due to the wave speed of λ_3 , therefore, for the corresponding cell the following time step is taken to advance the solution in time:

$$\Delta t_j = \Delta t_3 = \left| \frac{\Delta x_j}{u_j + c_j} \right| \quad (2.9)$$

where subscript j denote the node number. Usually a safety factor, less than one (say between 0.6 to 0.8), is applied to Δt_j to improve the stability of the solution.

2.3.1 Time-Accurate vs. Time-Inaccurate Schemes

In Section 2.2.5, it is noted that the governing equations for both steady and unsteady flows are intentionally written in unsteady form. For these unsteady equations two types of solutions are sought and are addressed in this section: (1) time-accurate and (2) time-inaccurate.

A solution is said to be time-accurate if it has a physically correct solution at any arbitrary time. This requires, first, the solution to be started from a physically correct initial condition and secondly a small enough time step to be taken for each step to give small truncation errors of the terms containing Δt . Thirdly, the solution in all the computational cells are advanced with a single time step value, which is the smallest Δt throughout the computational domain. This is referred to as a global time-step problem. This approach is suitable for physically unsteady problems, in which the history of the time integration is important.

Alternatively, in time-independent problems, the final converged solution is independent of initial conditions. Besides, the time steps could be taken as large as possible to quickly pass the transient region and to obtain the steady-state solution. Moreover, it is not required that the time step of all the computational cells be the same, i.e. the solution in each cell could advance by its own locally determined time-step. This is called a local time-step problem, which is used to accelerate the convergence of steady-state problems. In local time-step problems, the time-step may exhibit large variability throughout the computational domain. That is not

only due to the spatial variations of the wave speeds but also due to the size and shape of the computational cells, see Eqn. 2.8.

2.3.2 Implicit vs. Explicit Schemes

Time discretization of the fluid equations could be generally classified into two groups, explicit and implicit. Explicit methods compute the solution in the next time step directly based on the information in the current time (and/or previous times), which are known. Time steps in explicit schemes are not assigned arbitrarily but are limited by the stability criteria, see Eqn. 2.9. Therefore, explicit schemes may take more iteration steps to cover a given time than implicit schemes. Implicit schemes are more stable and they allow larger time steps to be taken to advance the solution in time and they can converge in fewer steps of iteration but the computational cost for each iteration is more. Larger time steps may however lead to sacrifice of accuracy in some problems.

Implicit schemes are somewhat more complicated to code than explicit schemes, because they require information provided during the time step for which the solution is being obtained. That is, the discretized equations for all the nodes are solved simultaneously. Explicit schemes are quite suitable for the time-accurate solutions, as outlined in Section 2.3.1, because time-accurate solutions require small time steps. On the other hand, the large time steps taken by implicit schemes produce a significant amount of truncation error for terms containing Δt . Implicit schemes require computationally expensive Jacobian matrices to be calculated for their implementation and this complication gets compounded when it involves upwind discretization, see Amaladas (1995); especially when higher order upwind schemes are implemented. With recent advancements in computational hardware, explicit schemes are able to give converged solutions within a reasonable period of time for engineering applications and the use of these schemes is justified.

Some of the important methods of the implicit time integration are approximately factored approach, (e.g. Beam and Warming (1978)), and relaxation techniques (Tannehill et. al. (1997)). In approximately factored schemes, basically, a

multidimensional problem involving more than one spatial variable is resolved into simpler multi one-dimensional factors, which are solved in sequence using a block tridiagonal matrix. Otherwise it would be necessary to invert a block penta-diagonal matrix, which is inefficient.

Relaxation techniques can be based on the un-factored form of the equations and could be either an explicit, point-iterative method as described for example by Anderson (1995), or an implicit, line Gauss-Seidel relaxation method as described for example by Thomas and Walters (1985).

2.3.3 Predictor-Corrector

The Lax-Wendroff two step explicit predictor-corrector time integration scheme is given below. This scheme gives second order accurate solutions in time, which is usually considered satisfactory for time-independent problems, in which only the final converged solution is of interest.

The predictor step provides the flow condition in an intermediate step $n + 1/2$.

$$\frac{Q^{n+1/2} - Q^n}{\Delta t/2} + \left(\frac{\partial F}{\partial x} \right)^n = 0 \quad (2.10)$$

Eqn. 2.10 gives $Q^{n+1/2}$ and all the primitive variables (p , ρ , u) at the time step $n + 1/2$. The predictor step is followed by the corrector step, which completes the integration. In the corrector step, a central differencing in time around $n + 1/2$ is implemented as follows:

$$\frac{Q^{n+1} - Q^n}{\Delta t} + \left(\frac{\partial F}{\partial x} \right)^{n+1/2} = 0 \quad (2.11)$$

Any type of space discretization could be used for the evaluation $\partial F/\partial x$ in Eqns. 2.10 and 2.11. The MacCormack scheme (1969) is a sub-set of the Lax-Wendroff scheme, which uses forward difference in one step and backward difference in the other. The net discretization in space is 2nd order. The MacCormack scheme (1969) was the most predominately used scheme in the 1970's. The MacCormack scheme which alternates between forward and backward difference approximations has a built in pseudo unsteadiness so it cannot attain to machine accuracy. But this is not true

for all schemes of the Lax-Wendroff family. For example if upwind differencing is used for the space discretization in Eqns. 2.10 and 2.11, there will be no pseudo unsteadiness in the method and machine accuracy is achievable.

2.3.4 Runge-Kutta

Jameson (1981) presented the following fourth order Runge-Kutta-like scheme for time integration. It gives a fourth order of temporal accuracy, even though many people use it for steady state calculations. The major advantage of Runge-Kutta schemes is that the storage of multiple time steps of information is not required, so that a small memory is adequate.

$$\begin{aligned} Q_j^{(0)} &= Q_j^n \\ Q_j^{(k)} &= Q_j^{(0)} + \alpha_k \Delta t \left(\frac{\partial Q}{\partial t} \right)^{(k-1)} \\ Q_j^{n+1} &= Q_j^{(4)} \end{aligned} \tag{2.12}$$

where $\partial Q/\partial t = -\partial F/\partial x$ from the governing equation of a one-dimensional flow (for the two-dimensional flow $\partial Q/\partial t = -(\partial F/\partial x + \partial G/\partial y)$), $\alpha_k = 1/(5 - k)$ and $k=1, 2, 3$, and 4.

2.4 Space Discretization

As opposed to time-discretization, in which the versatility of techniques are comparatively limited, spatial discretization techniques are very versatile.

In Section 2.2.2 the numerical schemes were broadly classified into two groups central and upwind, based on the spatial discretization of inviscid terms. In the current section it will be first shown why upwind schemes are preferred for the discretization of inviscid terms. This will be followed by more details on two major categories of upwind differencing schemes, namely Flux Vector splitting (FVS) and Flux Difference splitting (FDS) schemes. The formulae development of these two schemes, FVS and FDS, are included in Appendices A to D.

Reviewing again the fluid equations, they could be viewed as composed of inviscid (convective and pressure) and viscous (diffusive) terms. These equations are written in non-dimensional form in Cartesian coordinates as follows: (for simplicity the time-dependent terms are dropped here).

$$\underbrace{\frac{\partial F_{inv}^*}{\partial x^*} + \frac{\partial G_{inv}^*}{\partial y^*}}_{\text{convective \& pressure terms}} = \frac{1}{R_e} \underbrace{\left(\frac{\partial F_{vis}^*}{\partial x^*} + \frac{\partial G_{vis}^*}{\partial y^*} \right)}_{\text{diffusive terms}}, \quad (2.13)$$

where F_{inv} and G_{inv} are the inviscid fluxes, F_{vis} and G_{vis} are the viscous fluxes, R_e is the Reynolds number and the superscript * indicates that the corresponding parameter is non-dimensional. It is noted that Eqn. 2.13 is in general elliptic.

Noting that Reynolds number is the ratio of inertia forces to viscous forces, two ultimate limits for the Reynolds number are considered: (1) $R_e \rightarrow 0$ and (2) $R_e \rightarrow \infty$.

In case (1), the ratio of inertia forces to viscous forces are very small and Eqn. 2.13 reduces to an elliptic equation in which only the diffusive terms remains. In case (2), the ratio of inertia forces to viscous forces are very large and Eqn. 2.13 reduces to a hyperbolic equation in which only the convective and pressure terms remain. These two ultimate limits for the Reynolds number enlighten the choice for the discretization schemes.

The diffusive terms in Eqn. 2.13 are always discretized by central difference (as mentioned in Section 2.2.2). This is in accordance with the limit that $R_e \rightarrow 0$, which corresponds to the case for which viscous effects dominate.

On the other hand in the other limit, as $R_e \rightarrow \infty$ the fluid equations reduce to the Euler equations, in which inertial forces dominate. At this point two types of spatial discretization for the convective and pressure terms (inviscid fluxes) could be assumed:

(I) Central Difference (CD) schemes, in which a symmetric choice of the information stored in the neighboring nodes are used to obtain the numerical flux at the cell faces. By this choice, the typical essence of hyperbolic problems is lost.

(II) On the other hand, upwind schemes are designed on the basis of agreement with the physics of flow allowing for the direction from which the information arrives

at the cell face. This adds some confidence that a physically realistic numerical scheme is chosen.

More information about upwind schemes are given in Appendices A to D (covering a range from the wave equation, the solution of the decomposed form of the fluid equations, FVS and FDS as applied to fluid equations and the Roe scheme formulations in one and two dimensions).

Most of the upwind schemes can be grouped into three major categories as: (1) Exact Riemann Solver (ERS) schemes, (2) Flux Vector Splitting (FVS) schemes and (3) Approximate Riemann Solver (ARS) schemes.

For the higher order spatial discretization, as called high resolution, there are generally two types of approaches: (1) Monotone Upstream-centered Schemes for Conservation Laws (MUSCL), in which either the primitive variables or conservative variables are extrapolated to the cell faces by the desired order of accuracy and the inviscid fluxes are then determined directly at the cell faces and (2) the inviscid fluxes are determined at the nodes and are then extrapolated to the cell faces. In approach (1) the conservation laws are locally governed at the cell faces as recommended by van Leer (1979, 1982).

2.4.1 Exact Riemann Solver (ERS) Schemes

ERS schemes, sometimes known as Godunov type of schemes, solve the governing equations of fluid motion by distributing piecewise constant data over the flow field, which are analytically integrated in time to obtain the solution. This gives the distribution of data over each cell, which is obtained by an exact method. Then the new condition at each cell is approximated again by piecewise constant data. This strategy can be repeated until the desired solution is obtained. Since in the Godunov method the data are approximated by piecewise constant distribution, it is probably not worth seeking an exact solution for an approximate problem as it will not be a computationally efficient approach. Therefore, other alternative approaches are sought to solve the fluid equations.

2.4.2 Flux Vector Splitting (FVS) Schemes

Flux Vector Splitting for the Euler equations is a consequence of viewing the fluid particles, some of which are moving forward and others moving backward. This establishes the basis of splitting the fluxes of mass, momentum and energy into forward and backward components. The leading scheme of FVS type is due to Steger and Warming (1981), where Steger and Warming formulated the characteristics theory into conservation law form by splitting the flux vectors according to the sign of the eigenvalues of the Jacobian flux. It is noted that these eigenvalues are the speed of the traveling acoustic waves, see Appendix B, in which the characteristics form of the fluid equations are derived. As proven in Appendix B, the inviscid-flux vectors are a homogenous function of the conservative vector for perfect gases. Steger and Warming used this advantage and were able to split the inviscid flux vectors into positive (resembling particles moving forward) and negative terms (resembling particles moving backward). However, for real gases, the homogenous property of the inviscid fluxes are lost, therefore, the Steger-Warming method cannot be directly extended to real gases. Some approximations have been proposed to overcome this shortcoming, see Liou et. al. (1990) for example.

Another difficulty of the Steger and Warming method was encountered when the eigenvalues of the Jacobian fluxes vanish (the locus that characteristic speed passed through zero at sonic or stagnation points). This caused the derivatives of the split fluxes to be discontinuous, even for perfect gases. The difficulty was corrected by moving the positive and negative eigenvalues away from their vanishing locations, as proposed by van Leer (1982).

The Steger-Warming method was first developed to solve the Euler equations. This scheme is fairly dissipative and should not be used to solve Navier-Stokes equations, because it causes shear layers to become remarkably large due to the enhancement of the physical diffusion by non-physical intrinsic artificial diffusion. Some modifications to this problem are possible by arithmetically averaging the data at the left and right sides of the cell faces, as outlined by MacCormack (1995). A comparison of the computation of Navier-Stokes with some upwind schemes as

well as central schemes are performed by van Leer et. al. (1987), concluding that artificial thickening of the shear layers are due to the excessive diffusivity of the FVS schemes. Their study recommends the use of the Approximate Riemann Solver of Roe (1981) for the computation of Navier-Stokes as well as Euler equations.

2.4.3 Approximate Riemann Solver (ARS)

One alternative to bypass the ERS approach for the solution of the fluid equations, is to solve the Riemann problems approximately, i.e. by ARS. This approach is able to capture the important features of the Riemann problems without the need to seek a computationally costly exact method. This makes the ARS schemes very distinctive. These schemes are based on the non-iterative solution of the Riemann problems. The two most popular ARS schemes are due to Roe (1981) and Osher (1984). There are two important distinctions of the Roe scheme: (1) Roe's scheme involves determining the primitive variables at the cell faces by blending data stored on both sides of the cell faces with a density-based averaging, giving the so called *Roe's averaged condition*. (2) The method actually splits the flux difference vector in contrast to FVS schemes that split the flux vector itself (this is the reason that the Roe scheme is categorized as a Flux Difference Splitting (FDS) scheme). These two characteristics of the Roe scheme make it a very accurate tool for the Navier-Stokes as well as Euler computations. MacCormack (1995) noted that the Roe method is the method of choice today because of the above two properties. In addition a major reason for the popularity of the Roe scheme is its simplicity.

One major shortcoming of the Roe scheme is that it does not automatically satisfy the entropy condition. Therefore, expansion waves in sonic regions are captured as expansion shocks (as a completely unphysical phenomena). There are a variety of techniques to fix this problem. Some of these techniques are reviewed and benchmarked in Chapter 4 and a modification is also given there. This modification simply enlarges the band over which the entropy condition is applied by a factor of four. The modified formulae is able to totally remove the expansion shocks from the sonic expansion regions without influencing the rest of the computational domain.

Osher's scheme represents the flux difference as a path integral in space. This is integrated along a path which is piecewise aligned with the corresponding eigenvectors of the Jacobian matrix, see Amaladas (1995). Osher's scheme can automatically satisfy the entropy condition. However, its implementation is quite complicated.

The development of the formulae for the FVS and FDS schemes are given in Appendix C. This is followed by a complete formulation of the Roe scheme in one and two dimensions as given in Appendix D.

2.4.4 Time and Space Discretization in the Current Study

In the current study, an upwind, density-based, shock capturing explicit method is used to solve the fluid equations. For the spatial discretization of the inviscid terms three different approaches are studied:

1. Second order upwind scheme, in which the numerical oscillations are damped by minmod TVD. This approach is described in Chapter 4, in which the entropy fix condition as applied to the Roe scheme is modified. In this approach, second order accuracy is achieved by extrapolating primitive variables to the cell face by the MUSCL idea as proposed by van Leer (1979). To damp the spurious numerical oscillations, which is always needed in the spatial discretization techniques of more than first order accuracy, the minmod flux limiter is used.
2. Third order upwind-biased scheme is used as applied to the Roe scheme, in which the primitive variables are extrapolated to the cell faces by MUSCL idea. To damp the spurious numerical oscillations the van Albada (1982) flux limiter is used. This flux limiter is reported in two different forms in the literature, one of which converges faster. This advantage is explored by two independent and personal communications with Dr. J. L. Thomas of NASA Langley (2000) and Dr. J. R. Amaladas (2000) of Indian Institute of Science, India. The difference between these formulations are explained in Chapter 6.
3. Mixing the second and third order schemes by appropriate weight from each

of them has resulted in a non-oscillatory numerical algorithm with no flux limiter. In this approach, which is applied to the van Leer FVS scheme (1982), the fluxes at the nodal points are directly extrapolated to the cell faces rather than using the MUSCL extrapolation strategy. This approach as applied to two dimensional planar and axisymmetric flows is reported in Chapter 3.

The above-mentioned spatial discretization are only implemented for inviscid terms (see Eqn. 2.1) in the current study. For the spatial discretization of the viscous terms, central difference is always used.

For the temporal discretization, either Euler's first order forward, or second order two step predictor-corrector from the Lax-Wendroff family, as discussed in Section 2.3.3, is used. The governing equations are recast in generalized coordinates and are solved in these coordinates.

Figure 2.1: Cell j with boundaries at $j + \frac{1}{2}$ or E and $j - \frac{1}{2}$ or W .

Figure 2.2: Discontinuities of primitive variables (p , ρ , and u) through a normal shock as compared to a continuous profile of the flux parameters (ρu , $\rho u^2 + p$, etc.)

Chapter 3

Development of a Second Order Upwind Scheme with Application to Supersonic Euler Flow

3.1 Introduction

A second-order fully upwind scheme is developed and applied to the supersonic inviscid flow described by the Euler equations. The scheme is developed by combining the standard second- and third-order fully upwind schemes each with a specified appropriate weight. These weights are obtained by numerical simplification of the computational molecule and by numerical experiments. Both the standard second- and third-order schemes require a flux limiter to bound the unwanted numerical oscillations, without which they are unable to achieve the machine accuracy, $\approx \mathcal{O}(10^{-14})$. However, the current scheme requires no flux limiter for all the test cases performed and it is demonstrated to be accurate, robust and to give non-oscillatory results, attaining machine accuracy. Agreement between the results of the current study and the results obtained from the classical theory of oblique shocks is within an average error of 4% or better for all the cases examined.

Upwind schemes have been developed on the basis that information propagates in the physical domain, along characteristic directions which are determined, in math-

emational terminology, by the sign of the eigenvalues of the flux Jacobian. These eigenvalues are positive at a point at which the flow is locally one-dimensional supersonic, and are: V , $V + a$, and $V - a$ where V is the total velocity in the locally one-dimensional flow and a is the speed of sound. A positive eigenvalue at a point in the physical domain indicates that the physical properties at this point are dependent only on their upstream values. That is, the governing equations of fluid motion are hyperbolic for locally one-D supersonic flow. For a locally subsonic flow (say for simplicity still in the context of locally 1-D flow) with one negative eigenvalue, i.e. $V - a$, the physical properties at the point of interest are dependent on both downstream as well as upstream values. The flow is thus elliptically governed.

A numerical scheme for solving the flow equations should be consistent with the physics of the problem and should consider the characteristic directions in which information propagates in the physical domain. Such flows are better solved by upwind schemes as compared to central schemes.

High resolution schemes in the vicinity of sharp discontinuities usually exhibit oscillatory behavior, which is of purely numerical origin. To damp these oscillations, central difference schemes require both artificial viscosity and flux limiters. Upwind schemes do not require artificial diffusion. However, they usually require a flux limiter to damp the numerical oscillations in the vicinity of large gradients. One exception to this is the category of Essentially Non-Oscillatory (ENO) schemes (see Laney (1998) for example). ENO schemes are very complicated for modeling, therefore, for the higher resolution applications the traditional approach is preferred in which a flux limiter is added rather than using ENO without limiter.

In the present work, standard second- and third-order upwind schemes are combined each with appropriate weight, and the result is a non-oscillatory second-order upwind scheme which needs no flux-limiters even for flows with sharp discontinuities, such as shock waves. The method is not a type of the ENO schemes, which are very complicated to model, it is rather simple and is obtained by linearly blending the second and third order terms by appropriate weight applied to each. The method is applied to some inviscid compressible flows containing strong discontinuities, which are described by the Euler equations.

3.2 Governing Equations

The governing equations of fluid motion used here are the time-dependent compressible Euler equations in generalized coordinates. These equations in full conservative form are written as:

$$\frac{\partial \bar{Q}}{\partial t} + \frac{\partial \bar{F}}{\partial \xi} + \frac{\partial \bar{G}}{\partial \eta} + \alpha \bar{H} = 0 \quad (3.1)$$

where $\bar{Q}$ is the solution vector to be obtained. $\bar{F}$ and $\bar{G}$ are the ξ - and η - direction inviscid flux vectors and $\bar{H}$ is the inviscid source term, all written in generalized coordinates. For stationary grids, where grid configurations are time invariant, one can write (see Hoffmann and Chiang (1993) for example):

$$\bar{Q} = \frac{Q}{J}, \quad (3.2)$$

$$\bar{F} = \frac{1}{J} [\xi_x F + \xi_y G], \quad (3.3)$$

$$\bar{G} = \frac{1}{J} [\eta_x F + \eta_y G], \quad (3.4)$$

where:

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ E_t \end{bmatrix}, \quad F = \begin{bmatrix} \rho u \\ p + \rho u^2 \\ \rho uv \\ (E_t + p)u \end{bmatrix}, \quad G = \begin{bmatrix} \rho v \\ \rho uv \\ p + \rho v^2 \\ (E_t + p)v \end{bmatrix}, \quad H = \frac{1}{y} \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 \\ (E_t + p)v \end{bmatrix} \quad (3.5)$$

and ρ, p, T, u, v, E_t are density, pressure, temperature, x- and y-velocity components and the total energy per unit volume, respectively. E_t is the sum of the internal and kinetic energy per unit volume given by:

$$E_t = \rho \left(e + \frac{V^2}{2} \right) \quad (3.6)$$

where $V^2 = u^2 + v^2$ and e is the internal energy per unit mass. For a calorically perfect gas, pressure can be estimated by the equation of state:

$$p = \rho (\gamma - 1) e \quad (3.7)$$

where γ is the ratio of specific heats, which is constant for perfect gases with a value of 1.4 used here as applicable to air. Finally α is either 0 (for 2-D planar flow), or 1 (for 2-D axisymmetric flow). Both 2-D planar and axisymmetric flows are considered (see in Kermani and Plett (1998^a) and (1998^b)).

The convective and pressure terms of the Euler equations, $\bar{F}$ and $\bar{G}$, are split according to the Flux Vector Splitting (FVS) method of van Leer (1982) as explained for example in Hoffmann and Chiang (1993). These inviscid fluxes are split as follows: $\bar{F} \equiv \bar{F}^+ + \bar{F}^-$, and $\bar{G} \equiv \bar{G}^+ + \bar{G}^-$, where positive- and negative- fluxes correspond to positive- and negative-eigenvalues of the Jacobian matrices $\partial\bar{F}/\partial\bar{Q}$ and $\partial\bar{G}/\partial\bar{Q}$, respectively. These fluxes are differenced as follows:

$$\frac{\partial\bar{F}}{\partial\xi} = \frac{\partial(\bar{F}^+ + \bar{F}^-)}{\partial\xi} = \frac{D_- \bar{F}^+ + D_+ \bar{F}^-}{\Delta\xi} \quad (3.8)$$

$$\frac{\partial\bar{G}}{\partial\eta} = \frac{\partial(\bar{G}^+ + \bar{G}^-)}{\partial\eta} = \frac{D_- \bar{G}^+ + D_+ \bar{G}^-}{\Delta\eta} \quad (3.9)$$

where D_- denotes backward difference and D_+ denotes forward difference in space.

3.3 Spatial Differencing

Consider a grid distribution as shown in Fig. 3.1. Standard second- and third- order differencing for term $\partial F/\partial\xi$ could be written as:

$$\left(\frac{\partial F}{\partial\xi}\right)_{2^{nd}-order} = \Delta_2 + \mathcal{O}(\Delta\xi)^2 \quad (3.10)$$

$$\left(\frac{\partial F}{\partial\xi}\right)_{3^{rd}-order} = \Delta_3 + \mathcal{O}(\Delta\xi)^3 \quad (3.11)$$

where Δ_2 and Δ_3 are obtained from Taylor series expansions for fully upwind scheme:

$$\Delta_2 \equiv \frac{1}{2\Delta\xi} [3F_J - 4F_{J-1} + F_{J-2}] \quad (3.12)$$

and

$$\Delta_3 \equiv \frac{1}{6\Delta\xi} [11F_J - 18F_{J-1} + 9F_{J-2} - 2F_{J-3}] \quad (3.13)$$

The second- and third-order definition for the flux derivative are blended by contribution from each of them and a net value for the flux derivative could be defined:

$$\Delta_{net} \equiv W_1 \Delta_2 + W_2 \Delta_3 \quad (3.14)$$

or

$$\left(\frac{\partial F}{\partial \xi}\right)_{net} = W_1 \left(\frac{\partial F}{\partial \xi}\right)_{2^{nd}-order} + W_2 \left(\frac{\partial F}{\partial \xi}\right)_{3^{rd}-order} \quad (3.15)$$

where the sum of the weights has to be equal to one, i.e.

$$W_1 + W_2 = 1 \quad (3.16)$$

W_1 and $W_2 (= 1 - W_1)$ are selected by mathematical simplification of the computational molecule and numerical experiment. This issue is addressed next.

Selection of W_1 and W_2

Consider the node distribution along the string as shown in Fig. 3.2. The average values associated to each control volume is shown in this figure. $(\partial F / \partial \xi)_J$ for any degree of accuracy could be obtained by:

$$\left(\frac{\partial F}{\partial \xi}\right)_J = \frac{F_E - F_W}{\Delta \xi} \quad (3.17)$$

where by Taylor expansion it can be shown that

- for first order:

$$F_E^{(1)} = F_J, \quad (3.18)$$

- for second order upwind:

$$F_E^{(2)} = F_J + 0.5(F_J - F_{J-1}) = \frac{3}{2}F_J - \frac{1}{2}F_{J-1}, \quad (3.19)$$

- and for third order upwind:

$$F_E^{(3)} = \frac{11}{6}F_J - \frac{7}{6}F_{J-1} + \frac{1}{3}F_{J-2}, \quad (3.20)$$

where the superscript shows the degree of accuracy of the upwind scheme. The proposed numerical scheme (denoted by (net)) could be written as:

$$F_E^{(net)} = W_1 F_E^{(2)} + (1 - W_1) F_E^{(3)} \quad (3.21)$$

After substituting the values for the second and third order, one can obtain:

$$F_E^{(net)} = \frac{F_J}{6} [11 - 2W_1] - \frac{F_{J-1}}{6} [7 - 4W_1] + \frac{F_{J-2}}{3} [1 - W_1] \quad (3.22)$$

The choice of $W_1 = 1$ eliminates the last term of Eqn. 3.22 and reduces the scheme to a second order upwind scheme as given by Eqn 3.19. As expected this scheme needs flux limiter to damp the numerical oscillations. The choice of $W_1 = 0$, enhances the accuracy of the (net) scheme to third order upwind as given by Eqn. 6.6, which need a stronger flux limiter to damp the oscillations.

The appropriate selection algorithm for W_1 is performed first by simplification of the computational molecule by vanishing the coefficients of either F_J or F_{J-1} . This is followed by the numerical experiments to assess the accuracy in predicting the solutions.

1. Vanishing the coefficient of F_J leads to:

$$W_1 = \frac{11}{2} \quad W_2 = 1 - W_1 = -\frac{9}{2} \quad (3.23)$$

and in turn

$$F_E^{(net)} = \frac{5}{2} F_{J-1} - \frac{3}{2} F_{J-2} \quad (3.24)$$

and

2. Vanishing the coefficient of F_{J-1} leads to:

$$W_1 = \frac{7}{4} \quad W_2 = 1 - W_1 = -\frac{3}{4} \quad (3.25)$$

and in turn

$$F_E^{(net)} = \frac{5}{4} F_J - \frac{1}{4} F_{J-2} \quad (3.26)$$

If vanishing of the coefficient of F_J is chosen, there is no contribution from the nearest node (i.e. F_J) when F_E is sought. Also the weight of W_1 in this choice,

i.e. Choice 1, is stronger and has more potential of showing unstable behavior. Therefore, Choice 2 selected. Consequently the (net) upwind difference could be obtained as follows:

$$\left(\frac{\partial F}{\partial x}\right)_J^{(net)} = \frac{1}{4\Delta\xi} [5F_J - 5F_{J-1} - F_{J-2} + F_{J-3}] \quad (3.27)$$

The same results as given by Eqn. 3.27 could also be obtained by substituting $W_1 = 7/4$ and $W_2 = -3/4$ into Eqn. 3.15 with the values of the upwind differencing given by Eqns. 3.12 and 3.13.

Before performing any test to assess the performance of the proposed numerical scheme, it is appropriate to investigate its spatial accuracy. For an n^{th} order accurate scheme the polynomial of degree n (i.e. $F(\xi) = \xi^n$) should satisfy the difference equation. This is performed as follows:

- For $n = 0$, $F(\xi) = \xi^0 = 1$ and $dF/d\xi = 0$. This could be verified by:

$$\left(\frac{\partial F}{\partial x}\right)_J^{(net)} = \frac{1}{4\Delta\xi} [5(1) - 5(1) - 1 + 1] = 0 \quad O.K. \quad (3.28)$$

- For $n = 1$, $F(\xi) = \xi$ and $dF/d\xi = 1$. If the origin is taken at $J = 1$, thus $F_J = 0$, $F_{J-1} = -\Delta\xi$, $F_{J-2} = -2\Delta\xi$ and $F_{J-3} = -3\Delta\xi$. Therefore,

$$\left(\frac{\partial F}{\partial x}\right)_J^{(net)} = \frac{1}{4\Delta\xi} [5(0) - 5(-\Delta\xi) - 1(-2\Delta\xi) + 1(-3\Delta\xi)] = \frac{4\Delta\xi}{4\Delta\xi} = 1 \quad O.K. \quad (3.29)$$

- For $n = 2$, $F(\xi) = \xi^2$, $dF/d\xi = 2\xi$ and at $\xi = 0$, $dF/d\xi = 0$. This could be checked by substituting for $F_J = 0$, $F_{J-1} = (-\Delta\xi)^2 = (\Delta\xi)^2$, $F_{J-2} = (-2\Delta\xi)^2 = 4(\Delta\xi)^2$ and $F_{J-3} = (-3\Delta\xi)^2 = 9(\Delta\xi)^2$

$$\left(\frac{\partial F}{\partial x}\right)_J^{(net)} = \frac{1}{4\Delta\xi} [5(0) - 5(\Delta\xi^2) - 1(4\Delta\xi^2) + 1(9\Delta\xi^2)] = \frac{0}{4\Delta\xi} = 0 \quad O.K. \quad (3.30)$$

Later it will be shown that the polynomial of degree $n = 3$ does not satisfy the proposed scheme. Therefore, the proposed numerical scheme, as indicated by (net), is spatially second order.

Numerical experiments with a set of values selected for W_1 and W_2 have been performed. The values are: $W_1 = 1, W_2 = 0$, which gives the standard second order accurate formulation as given by Eqn. 3.12. Similarly, $W_1 = 0, W_2 = 1$, which gives the third order upwind scheme as given by Eqn. 3.13, $W_1 = 1/2, W_2 = 1/2$, which could be viewed as Crank-Nicolson type of averaging and $W_1 = 7/4, W_2 = -3/4$, which is the proposed scheme as denoted by superscript (net) here. With all values given here for W_1 and W_2 a flux limiter is needed, except for $W_1 = 7/4, W_2 = -3/4$, which does not require a flux limiter.

One possible way to justify this, could be what is proposed as follows. If a polynomial of degree $n = 3$ is attempted by the second order upwind scheme as given by Eqn. 3.12 and by the currently proposed scheme, (net), this could elaborate on this matter.

For $n = 3$, $F(\xi) = \xi^3$, $dF/d\xi = 3\xi^2$ and at $\xi = 0$, $dF/d\xi = 0$. By setting the origin at $J = 1$, $F_J = 0$, $F_{J-1} = (-\Delta\xi)^3 = -(\Delta\xi)^3$, $F_{J-2} = (-2\Delta\xi)^3 = -8(\Delta\xi)^3$ and $F_{J-3} = (-3\Delta\xi)^3 = -27(\Delta\xi)^3$. The first term of the truncation error of the second order upwind scheme (see Eqn. 3.12) for a third order polynomial of the form $F = \xi^3$ could be determined as:

$$\left(\frac{\partial F}{\partial x}\right)_J^{(2)} = \frac{1}{2\Delta\xi}[3(0) - 4(-\Delta\xi^3) + 1(-8\Delta\xi^3)] = -2(\Delta\xi)^2, \quad (3.31)$$

and for the (net) scheme:

$$\left(\frac{\partial F}{\partial x}\right)_J^{(net)} = \frac{1}{4\Delta\xi}[5(0) - 5(-\Delta\xi^3) - 1(-8\Delta\xi^3) + 1(-27\Delta\xi^3)] = -3.5(\Delta\xi)^2. \quad (3.32)$$

According to Eqns. 3.31 and 3.32 the magnitude of truncation error for a given $\Delta\xi$ obtained from the standard second order upwind scheme is 7/4 times smaller than that of the net scheme. This does not mean that the proposed scheme is less accurate than a second order scheme. However, having a rate of diminishing less than a standard second order accuracy, introduces an excessive truncation error as compared to standard second order upwind scheme and this could be the reason that the proposed scheme needs no flux limiter to damp the oscillations.

Each set of W_1 and W_2 has been applied to the flow solver, which is an inviscid compressible Euler flow solver developed based on the FVS of van Leer (1982), and

the level of accuracy and convergence which is attainable has been investigated.

To show the behavior of the current scheme and to compare its performance with the performances of the standard second- and third-order upwind schemes the residuals of the governing equations of the fluid motion, Eqn. 3.1, are defined as:

$$R \equiv -\Delta t \left(\frac{\partial \bar{F}}{\partial \xi} + \frac{\partial \bar{G}}{\partial \eta} \right) \quad (3.33)$$

and the rates at which R diminishes as the solution marches in time and the solution approaches the steady state are studied.

The flux derivatives Δ_{net} (i.e., $W_1 = 7/4$ and $W_2 = -3/4$), Δ_2 (i.e., $W_1 = 1$ and $W_2 = 0$), and Δ_3 (i.e., $W_1 = 0$ and $W_2 = 1$) as approximations for the flux derivatives, are used in turn to evaluate Eqn. 3.33. With Δ_2 , accuracy of only $\mathcal{O}(10^{-3})$ is achievable, after which the oscillatory solutions grow and then diverge. With Δ_3 it is worse and growing oscillatory solutions start immediately from the beginning of computations as shown in the Fig. 3.3. However, with the currently proposed scheme, Δ_{net} , the machine accuracy is achievable and the solver converges to the machines accuracy $\mathcal{O}(10^{-14})$ when run in double precision (Fig. 3.4).

Interestingly, for all the test cases performed in this thesis, which will be discussed in section 3.5, the values of W_1 ($=7/4$) and W_2 ($=-3/4$) are not re-tuned. Agreement with classical solutions for all the cases considered is within 4%.

It should also be noted that, the accuracy of the proposed numerical scheme is unified throughout the computational domain and is not needed to be reduced in the vicinity of shock waves as opposed to a standard high resolution schemes which employ a flux limiter to reduce the slope of extrapolation in the region of large gradients.

As for the van Leer FVS scheme the split inviscid fluxes ($F = F^+ + F^-$) are needed, therefore, the positive and negative derivatives of the scheme (net) are written. That is:

$$\Delta_{net}^- = \frac{-\bar{F}_{J+3}^- + \bar{F}_{J+2}^- + 5\bar{F}_{J+1}^- - 5\bar{F}_J^-}{4\Delta\xi}. \quad (3.34)$$

and

$$\Delta_{net}^+ = \frac{5\bar{F}_J^+ - 5\bar{F}_{J-1}^+ - \bar{F}_{J-2}^+ + \bar{F}_{J-3}^+}{4\Delta\xi}. \quad (3.35)$$

3.4 Boundary Conditions

At the inlet face of the computational domain, where supersonic flow enters the domain of calculation, all flow variables are specified. At the exit, where supersonic flow leaves the domain of calculation, extrapolation from the interior nodes are performed to find the values at the exit face.

At the surface of the body, boundary conditions consistent with the Euler equations are applied. The normal component of velocity is set to zero. This is the only physically given boundary condition at the surface of the body. To determine other flow properties at the surface of the body, such as pressure, temperature, etc., the governing equations of fluid motion must be solved with one sided extrapolation to the wall. However, sometimes this is costly in terms of computational time. Therefore other approximations are sought.

Surface pressure is determined by solving the normal momentum equation. Tangential velocity at the surface of the body is extrapolated from interior nodes. Total enthalpy at the surface is set to the free stream total enthalpy. This is consistent with the energy equation in Euler flow, $\rho \frac{DH_t}{Dt} = \frac{\partial P}{\partial t}$, as the steady state condition approaches (see Hoffmann and Chiang (1993)), where H_t is the total enthalpy. This condition implies that total temperature at the surface is set to the free stream stagnation temperature. This is an exact equation for inviscid steady flows since there is no means of heat transfer from outside of the computational domain into the flow field (in terms of molecular collision analogy). However, it is only an approximation for the unsteady inviscid flows, since pressure is varying with time. In the current studies, in which steady-state solutions are sought by unsteady time marching, total enthalpy of the solid boundary and free stream have been equated.

Also, in the solution described herein, the computational domain is extended a distance upstream of the leading edge to permit the flow to adjust itself before reaching the body. Along this extension line, symmetry boundary conditions are

applied, which are $v = 0$ and $\frac{\partial S}{\partial y} = 0$, where

$$S = \begin{bmatrix} p \\ u \\ T \end{bmatrix}$$

The same boundary condition for 2-D planar and axisymmetric flows are applied.

3.5 Results and Discussion

3.5.1 Supersonic Flow Over a 10° Wedge

Supersonic inviscid flow with free stream Mach numbers, $M_1 = 2, 3.6$, and 5 , flowing over a 10° wedge is studied by the current numerical scheme, and the results are compared with the analytical results obtained from the Theory of Oblique Shocks (TOS).

Figure 3.5 shows an attached oblique shock over a compression corner. P_2 is the pressure downstream of the shock, θ is the deflection angle and β is the shock angle. Figure 3.6 shows the grid configuration for this flow analysis. This test is performed with a grid of 71×61 with the clustering factor of 1.2 . Figures 3.7, 3.8, and 3.9 show the pressure contours, isobar lines, for $M_1 = 2, 3.6$, and 5 , respectively, obtained from the current upwind scheme. These results together with their corresponding analytical results obtained from the TOS are compared in Table 3.1.

As can be seen from Table 3.2, agreement between the computation by the current scheme with the analytical results obtained from TOS is within an average error of 1.50 to 3.60% .

3.5.2 Shock Reflection from a Solid Boundary

The reflection of an oblique shock wave from a solid boundary is another test case, which is considered here. The schematic of the geometry is depicted in Fig. 3.10. in which a wedge with the angle θ and a horizontal wall above the wedge is shown.

The wedge deflects the flow by θ at point A , where an oblique shock is generated with the wave angle β_1 , incident shock. This causes flow to be deflected upward by the wedge angle θ . The incident shock impinges on the upper wall at point B and reflects to the main domain, as indicated by the reflected shock. This causes the flow in Region 2 to turn $-\theta$ to be parallel to the upper wall in Region 3.

This result is obtained on 71×61 uniform grids as shown in Fig. 3.11. Fig. 3.12 shows pressure contours together with the velocity vectors for flow conditions of $M_1=2$, and $\theta = 10^\circ$. Figure 3.13 is the enlargement of Fig. 3.12 near the impingement point B on the upper wall. As predicted by the TOS, velocity vectors in regions 1 and 3 are parallel to the upper wall, see Figs. 3.10, 3.12 and 3.13, and in Region 2 flow is parallel to the lower wall.

Table 3.3 shows the calculated values of β_1 , M_2 , $\frac{p_2}{p_1}$, $\frac{p_3}{p_1}$, M_3 , and Φ from the current study together with their corresponding analytical values from TOS.

Again, as shown in Table 3.3, the numerical computation is in good agreement with TOS results, with an average error of $\approx 2.5\%$.

3.5.3 Supersonic Diffuser

For the last case of 2-D planar flow, a supersonic two-dimensional diffuser with $M_1 = 2$ with angle $\theta = 10^\circ$ is studied (see Fig. 3.14). Shock generation from the compression corners at the top and the bottom of the computational domain, expansion waves, and multiple shock reflections from the solid walls are observed.

No analytical results were determined to compare the details of the current test. However, as can be seen from Fig. 3.14 the shock angle at the leading edge of the diffuser is $\tan^{-1} \frac{0.5/2}{0.3} \approx 39.81^\circ$. This agrees well with the result of TOS, of 39.20° .

3.5.4 Supersonic Axisymmetric Flow over a Cone

In the current section the method as described in this chapter is extended to axisymmetric flows, in which an inviscid supersonic flow over a 40 degree sharp cone (20 degree half-cone) is studied (see Kermani and Plett (1998^b) for more detail).

For this test case, various grid configurations are tested. Among them are: an

algebraic grid with or without clustering near the boundaries, and an orthogonal grid. The orthogonal grid configuration (61×61) is shown in Fig. 3.15 as an example.

The Mach number of the approaching flow is $M=2.00$. The results are shown in Fig. 3.16. Agreement with the results of Taylor-Macoll solution, (see Anderson (1995) for example), is within 4% difference. As seen earlier in this chapter for the 2-D planar case, streamlines downstream of the shock are parallel to the surface of the wedge. This can be seen in Fig. 3.12. However, for the axisymmetric flow over the cone, as predicted by the Taylor-Macoll solution, the streamlines downstream of the shock wave are not parallel to the surface of the cone. Such a phenomena can be observed in Fig. 3.16.

3.6 Concluding Remarks

A second-order upwind numerical differencing scheme is developed and applied to 2-D planar and axisymmetric flows over a variety of geometries. Agreement between the numerically predicted results and the results obtained from the classical theory of oblique shock waves is within an average error of 4% or better for the cases examined.

The values for the weighting functions, $W_1 = 7/4$ and $W_2 = 1 - W_1 = -3/4$ for all the tested 2- dimensional planar and axisymmetric cases have not been re-tuned and no flux-limiter has been added to damp the oscillations.

Table 3.1: Comparison of the pressure ratio between (1) current calculation and (2) analytical methods for the supersonic flow over the wedge.

M_1	$(\frac{p_2}{p_1})_{cal.}^a$	$(\frac{p_2}{p_1})_{anl.}^b$	$error_1$
2	1.69	1.71	1.17%
3.6	2.22	2.31	3.90%
5	3.22	3.04	-5.92%

M_1	$\beta_{cal.}$	$\beta_{anl.}$	$error_2$
2	38.70	39.31	1.55%
3.6	23.75	23.90	0.63%
5	18.78	19.38	3.10%

M_1	$M_{2cal.}$	$M_{2anl.}$	$error_3$
2	1.61	1.64	1.83%
3.6	3.02	2.98	-1.34%
5	4.07	4.00	-1.75%

^acal.: calculated by the current scheme.

^banl.: analytical results from TOS.

Table 3.2: Error between the (1) current calculation and (2) analytical methods for supersonic flow over the wedge.

M_1	Av. error ^a
2	1.52%
3.6	1.96%
5	3.59%

^aAv. error = $\frac{1}{3} \sum_{i=1}^3 |error_i|$

Table 3.3: Comparison between (1) the current calculation and (2) analytical methods for the shock reflection from the solid boundary.

$\beta_{1_{cal.}}^a$	$\beta_{1_{anl.}}^b$	$error_1$
39.50	39.20	-0.77%
$M_{2_{cal.}}$	$M_{2_{anl.}}$	$error_2$
1.64	1.65	0.61%
$\left(\frac{p_2}{p_1}\right)_{cal.}$	$\left(\frac{p_2}{p_1}\right)_{anl.}$	$error_3$
1.60	1.69	5.33%
$\left(\frac{p_3}{p_1}\right)_{cal.}$	$\left(\frac{p_3}{p_1}\right)_{anl.}$	$error_4$
2.69	2.80	3.93%
$M_{3_{cal.}}$	$M_{3_{anl.}}$	$error_5$
1.28	1.29	0.78%
$\Phi_{cal.}$	$\Phi_{anl.}$	$error_6$
40.40	39.00	-3.59%

^acal.: calculated by the current scheme.

^banl.: analytical results from TOS.

$$Av. error = \frac{1}{6} \sum_{i=1}^6 |error_i| = 2.50\%$$

Figure 3.1: Uniform grid distribution in Computational domain.

Figure 3.2: Node distribution along a one-dimensional string with the average values associated to each control volume.

Figure 3.3: Third order fully upwind, Δ_3 , residuals determined for supersonic flow of $M = 5.0$ over the 10° wedge as an example. It shows the residuals of all the governing equations, i.e., continuity-, x- and y-momentum, and energy-equations, grow immediately from the beginning of computations.

Figure 3.4: Continuity-, x- and y-momentum, and energy- equations residuals determined by the current scheme, Δ_{net} , for supersonic flow of $M = 5.0$ over the 10° wedge. All the residuals converge to the machine accuracy, $\mathcal{O}(10^{-14})$.

Figure 3.5: Supersonic flow over a wedge.

Figure 3.6: Grid configuration applied for supersonic flow over the wedge.

Figure 3.7: Supersonic flow with free stream $Mach = 2$ over a 10° wedge. $\beta_{cal.} = 38.7^\circ$ by the current scheme and $\beta_{ant.} = 39.2^\circ$ from TOS.

Figure 3.8: Supersonic flow with free stream $Mach = 3.6$ over a 10° wedge. $\beta_{cal.} = 23.75^\circ$ by the current scheme and $\beta_{ant.} = 24^\circ$ from TOS.

Figure 3.9: Supersonic flow with free stream $Mach = 5$ over a 10° wedge. $\beta_{cal.} = 18.78^\circ$ by the current scheme and $\beta_{ant.} = 19.5^\circ$ from TOS.

Figure 3.10: Reflection of shock wave from a solid boundary.

Figure 3.11: Grid configuration for flow over a 10° wedge, with 71×61 uniform grids.

Figure 3.12: Isobar lines and velocity vectors for supersonic flow with shock reflection from a solid boundary. $\Phi_{cal.} = 40.4^\circ$ by the current scheme and $\Phi_{anl.} = 39^\circ$, where Φ is the angle between the top plate and the reflected shock.

Figure 3.13: Enlargement of flow configuration near the impingement point of previous figure.

Figure 3.14: Pressure contours for a supersonic diffuser containing shocks, expansion waves, and multiple shock reflections from the solid boundaries.

Figure 3.15: Orthogonal grid configuration for a 20 degree half cone.

Figure 3.16: Iso-bar lines with streamlines for flow over a 20 degree half cone (40 degree total). Free stream Mach no= 2.00, Agreement with Taylor-Macoll solution is within 4% difference.

Chapter 4

Modified Entropy Correction Formula for the Roe Scheme

4.1 Introduction

To avoid unrealistic solutions like expansion shocks from appearing as a part of a solution, it is necessary to satisfy the entropy condition for the Roe scheme. A variety of entropy fix formulae for the Roe scheme have been addressed in the literature. Two of the popular ones are due to Harten-Hyman (1983) and one due to Hoffmann-Chiang (1993). These formulations have been assessed in this chapter by applying them to the inviscid Burgers' equation and the shock tube problem. These entropy fix formulations are unable to totally diminish the expansion shock in the vicinity of sonic expansions. Moreover, they are not universal, i.e. a single formulation is not adequate for the scalar Burgers' equation, shock tube problem and multi-dimensional cases. Therefore, the formulations must be re-tuned for different applications. A simple modification to the Harten-Hyman formulation is presented in this chapter. This modification basically enlarges the band over which the entropy fix condition is enforced. The modified formula is able to totally remove the non-physical expansion shocks from the region of sonic expansion without affecting the rest of the computational domain.

Comparisons among the exact solutions, with the formulae of Harten-Hyman,

Hoffmann-Chiang and the currently modified formula are shown here. The modified entropy fix formulation can totally diffuse the expansion shock. Moreover, the current formula does not affect the solution in the rest of the computational domain. In addition, the modified formula, as a single formulation, can universally be applied over a wide range of applications from scalar equations to fluid equations. Finally in this chapter, the following test cases are performed to assess the accuracy of the modified entropy formulation: inviscid shear flow, transonic flow over a bump, and transonic flow in a nozzle. Very accurate results are obtained.

In this chapter, the spatial discretization of the inviscid fluxes are performed by the second order upwind scheme of Roe with minmod flux limiter. For the time integration, a second order two step predictor-corrector of the Lax-Wendroff family is used. All the governing equations are solved within the framework of generalized coordinates.

4.2 Problem Definition; the Need for an Entropy Fix for the Roe Scheme

A scalar Riemann problem, such as the inviscid Burgers' equation subject to an initial condition with discontinuity, could easily be solved by an Exact Riemann Solver (ERS) like the Godunov method. However, when an ERS is applied to fluid equations, it gives a computationally inefficient iterative technique. For example, consider the governing equation of unsteady fluid motion for a one-dimensional flow, like the shock tube problem. This equation can be expressed in a fully conservative form as follows:

$$\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} = 0 \quad (4.1)$$

where t is time, x is space, Q is the solution vector, and F is the flux vector. This equation introduces a non-linear set of three coupled scalar equations for the one-dimensional case. Solving these equations by any type of iterative exact method, such as the ERS, is not computationally efficient.

One alternative idea that has been successfully used is to employ Approximate Riemann Solvers (ARS) for the fluid equations. One of the most popular ARS, is due to Roe (1981). The ARS of Roe (1981) suggests solving the linearized form of Eqn. 4.1, i.e.

$$\frac{\partial Q}{\partial t} + \bar{A} \frac{\partial Q}{\partial x} = 0 \quad (4.2)$$

where according to Roe (1981), $\bar{A}$ is a locally constant matrix and is determined in the so called *Roe's averaged condition* and satisfies certain conditions which Roe termed *property U*.

Since $\bar{A}$ in Eqn. 4.2 is locally constant, discrete expansion waves could appear as a non-physical process such as an expansion shock. The reason for the generation of this expansion shock in the Roe scheme can be better explained if the scheme is applied to the inviscid Burgers' equation. The Burgers' equation may be written as:

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left(\frac{u^2}{2} \right) = 0 \quad (4.3)$$

when Roe's linearization method is applied, Eqn. 4.3 will take the form:

$$\frac{\partial u}{\partial t} + \bar{u} \frac{\partial u}{\partial x} = 0 \quad (4.4)$$

where $\bar{u}$ is locally constant according to Roe (1981). Therefore, the solution of Eqn. 4.4 in each locality is equivalent to the solution of the wave equation (see Appendix A for the physical and numerical solutions of the wave equation):

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0 \quad (4.5)$$

where a is the wave speed. In fact, the wave equation, Eqn. 4.5, exactly reproduces the initial data at a distance $a \cdot t$ from its original location, where t is the time elapsed. That is, the initial data without any damping, amplification or any other change has been reproduced. For the case where it is possible that the wave speed a would vanish, Eqn. 4.5 would reduce to $\partial u / \partial t = 0$, for which the solution would be $u = \text{constant}$. That is, the initial data would be faithfully reproduced in its original location for any other time.

The linearized Burgers' equation, Eqn. 4.4, behaves exactly like the wave equation because $\bar{u}$ is locally constant. For the case that $\bar{u}$ vanishes, the initial data regardless of its configuration whether it is a compression or expansion, is faithfully reproduced. In other words, the linearized Burgers' equation, Eqn. 4.4, is not able to distinguish between a compression or expansion wave, since each is a valid solution of Eqn. 4.4. However an expansion shock is not a valid solution of the original Burgers' equation, Eqn. 4.3, and the correct physical solution is that the initial expansion condition must totally diffuse to a centered fan around the point of expansion. The existence of expansion shocks is a violation of the second law of thermodynamics, since it implies entropy reduction. This is corrected as shown in the following.

4.3 Entropy Correction

Later in this chapter, it will be shown that the Roe scheme is fairly non-diffusive for grid aligned flows and for oblique grids the amount of diffusion is very low. Therefore, it is very suitable for the computation of viscous flows, by which the viscous regions could be computed with a minimum artificial thickening of the shear layers, e.g. boundary layers. However, in the computations of inviscid flows some non-physical solutions such as expansion shocks may occur [Hirsch (1990), Tannehill et. al. (1997), and Hoffmann and Chiang (1993)] due to the lack of enough diffusivity. A very good catalog of the problems caused by the non-diffusivity characteristic of the Roe scheme is given by Quirk (1994).

The non-physical expansion shocks can occur in those regions of the computational domain in which expansions are observed through sonic regions, i.e. *sonic expansion*. In the case of Burgers' equation this occurs in the vicinity of $\bar{u}=0$. In order to remedy this problem it is required that: (1)- the location of the sonic expansion in the domain of computation is detected, and (2)- the expansion shock is avoided by diffusing the expansion shocks into expansion fans in the region of sonic expansion. Procedures (1) and (2) together are referred to as *entropy correction* or *entropy fix*.

(1)- Sonic expansion corresponds to the regions where the wave speed vanishes.

As mentioned earlier, for the Burgers' equation, this happens in the locality of $\bar{u} \approx 0$. For the one-dimensional flow, e.g. shock tube problem, the governing equations of fluid motion could be decomposed into an equivalent system with three scalar equations each being similar to the wave equation (see Appendix B for more detail):

$$\begin{aligned}\frac{\partial w_1}{\partial t} + \lambda_1 \frac{\partial w_1}{\partial x} &= 0, \\ \frac{\partial w_2}{\partial t} + \lambda_2 \frac{\partial w_2}{\partial x} &= 0, \\ \frac{\partial w_3}{\partial t} + \lambda_3 \frac{\partial w_3}{\partial x} &= 0,\end{aligned}\tag{4.6}$$

where w_1 , w_2 , and w_3 are *Riemann invariants*, which are constant along characteristic lines $dx/dt = \lambda_1$, λ_2 or λ_3 and $\lambda_1 = u - c$, $\lambda_2 = u$ and $\lambda_3 = u + c$ are the eigenvalues of the flux Jacobian matrix or the wave speed. For the one-dimensional flow, the regions of sonic expansion could be detected by searching the regions in which $|\lambda|$ approaches zero, or $|\lambda| < \epsilon$, where ϵ is a small and positive number which is carefully determined. In fact ϵ is the size of the band over which the entropy correction is enforced.

(2)- Once the region of sonic expansion is detected, an expansion shock can be avoided by diffusing the expansion shock into the domain of computation within the band ϵ .

The diffusion process is accomplished numerically by moving λ away from its origin. Various formulations could be used to diffuse the expansion shock. The most popular is due to Harten and Hyman (1983), which maps λ to:

$$\lambda_{new} \leftarrow \frac{\lambda^2 + \epsilon^2}{2\epsilon}.\tag{4.7}$$

For example, for $\epsilon = 0.5$ and $\lambda = 0$, the mapping of Eqn. 4.7 moves λ from its origin to $\lambda_{new} = 0.25$. Some of the popularly used entropy correction formulations are given next.

4.3.1 Accuracy Assessment of Entropy Correction Formulae

In the following entropy correction formulations it should be noted that $\hat{\lambda}$ is the eigenvalue determined at the Roe's averaged condition, e.g. $\hat{\lambda}_1 = \hat{u} - \hat{c}$. Also

$\lambda^L = u^L - c^L$ and $\lambda^R = u^R - c^R$ are the inner (L) and outer (R) values of the eigenvalue, respectively.

1. Harten and Hyman (1983)

$$\begin{cases} \hat{\lambda}_{new} \leftarrow \frac{\hat{\lambda}^2 + \epsilon^2}{2\epsilon} & |\lambda| < \epsilon \\ \epsilon = \max \left[0, (\hat{\lambda} - \lambda^L), (\lambda^R - \hat{\lambda}) \right], \end{cases} \quad (4.8)$$

2. Harten and Hyman (1983)

$$\begin{cases} \hat{\lambda}_{new} \leftarrow \epsilon & |\lambda| < \epsilon \\ \epsilon = \max \left[0, (\hat{\lambda} - \lambda^L), (\lambda^R - \hat{\lambda}) \right], \end{cases} \quad (4.9)$$

3. Hoffmann and Chiang (1993)

$$\begin{cases} \hat{\lambda}_{new} \leftarrow \frac{\hat{\lambda}^2 + \epsilon^2}{2\epsilon} & |\lambda| < \epsilon \\ 0 \leq \epsilon \leq 0.125 \end{cases} \quad (4.10)$$

Each of the entropy correction formulations (1) to (3) is applied to some determining test cases. The test cases used here are: (i) the scalar inviscid Burgers' equation subject to an initial expansion shock and, (ii) the shock tube problem. These are some of the standard test cases for which there is an exact solution available. Therefore, the numerical algorithms can be carefully assessed depending on how their solutions agree with the exact solution.

4.3.2 Inviscid Burgers' Equation

As the first test, the Roe scheme is applied to the inviscid Burgers' equations. The Burgers' equation is a hyperbolic equation in time, needing an initial condition to advance the solution in time. This initial condition is sketched in Fig. 4.1 which represents a sonic-expansion. A physically correct solution has to diffuse the initial condition into a centered expansion fan. However, the solution of the Burgers'

equation subject to this initial condition is predicted as an expansion shock by the Roe scheme, see Fig. 4.2-b. Therefore, the problem becomes a determining test to assess the accuracy of the entropy correction formulae (1) to (3). In this study, the computation is performed with various grid densities. However, the results presented here are with 81 grids along the x -axis.

The exact solution for this problem is shown in Fig. 4.2-a at time $t = 1.0$ sec. It shows that the initial sonic-expansion is totally diffused as a centered fan around the point of expansion, i.e $x = 2.0$. Fig. 4.2-b shows the Roe's scheme prediction, at iteration 81, equivalent to $t = 1.0$ sec, when no entropy correction is blended to the scheme. As shown in this figure the initial condition is faithfully repeated as the solution is advanced in time. This is a physically incorrect solution, which makes the enforcement of an appropriate entropy correction formula necessary for fixing the problem.

Entropy correction formula (1) partially diffuses the expansion shock as shown in Fig. 4.2-c. However, a small expansion shock still remains at the center of the expansion fan. Entropy correction formula (2) reduces the size of the expansion shock. However the shock has not totally disappeared as shown in Fig. 4.2-d, although it shows improvement over formulae (1).

Entropy formula (3) which uses a fixed band to impose the entropy correction, in this example $\epsilon = 0.1$, is not recommended because it produces a rather large expansion shock, as shown in Fig. 4.2-e. Entropy correction formulae (1) to (3) are applied to the shock tube problem next.

Entropy correction formula (4), i.e. the modified entropy correction formula as proposed in this chapter, is explained later in this chapter.

4.3.3 The shock Tube Problem

The next test case of the family of Riemann problems, is the shock tube problem. It contains all the challenging elements of fluid flow, which makes it very suitable for assessing the predictability of the numerical schemes. These elements in particular are: shock waves, contact discontinuities, and expansion waves in an unsteady frame

of reference as shown in Fig. 4.3.

The shock tube problem is an initial value problem. Therefore, as for the Burgers' equation, initial conditions are required. The initial conditions for this example are: $p^L = 10^5 \text{ Pa}$, $\rho^L = 1 \frac{\text{kg}}{\text{m}^3}$, $p^R = 10^3 \text{ Pa}$, $\rho^R = 0.01 \frac{\text{kg}}{\text{m}^3}$, and $u^L = u^R = 0$, where p , ρ , and u denote pressure, density and velocity respectively and index L and R refer to the fluid properties in the left and right side of the shock tube. The L and R sides are firstly separated by a diaphragm, which breaks at time $t = 0 \text{ sec}$, as depicted in Fig. 4.3. The initial conditions (the L and R flow properties at $t = 0 \text{ sec}$) are chosen in a way to give sonic regions as the solution develops in time. This will allow us to examine the performance of the entropy fix formulae in the sonic expansion regions. In this study, the computation is performed with various grid densities. However, the results presented here are with 101 grids along the tube.

Fig. 4.4 shows the Mach number distribution at $t = 3.9 \text{ milli sec}$ after the diaphragm is broken. Fig. 4.4-a shows the Mach number distribution obtained by the exact solution. As seen in this figure, there is no expansion shock at the point of sonic-expansion, i.e $Mach = 1.0$, and there is only a centered expansion fan.

Fig. 4.4-b shows the result with the Roe scheme with no entropy correction. This figure shows an expansion-shock occurring at the sonic point, which makes the enforcement of entropy corrections necessary.

Entropy correction formula (1) partially diffuses the expansion shock as shown in Fig. 4.4-c. However, an expansion shock still remains at the center of the expansion fan. Entropy correction formula (2) reduces the size of the expansion shock. However the shock has not yet totally diminished as shown in Fig. 4.4-d. Entropy formula (3) uses a fixed band for entropy correction, with $\epsilon = 0.1$, and produces a significantly larger expansion shock, as shown in Fig. 4.2-e.

The entropy correction formula (4) as developed in this chapter is applied to these test cases and its accuracy assessment is given next.

4.3.4 Proposed Entropy Correction Formulations

Although, the entropy correction formulations given in the previous section can partially diffuse the expansion-shocks and convert them to expansion fans, they cannot totally diminish the expansion shocks. Moreover, none of them is universal so that a single formulation is not applicable to a wide range of test cases from the inviscid Burgers' equation to the fluid equations like the shock tube problem or multidimensional cases as explained by Kermani and Plett (2001^a). A simple modification is applied to that of the Harten and Hyman (1983) entropy correction and a new formulation is proposed. The modified formula, can be applied to a wide range of problems and it can totally diffuse the expansion shocks in sonic regions into an expansion fan without influencing the rest of the computational domain. This is formulated as follows.

Entropy Correction Formula 4

The proposed entropy correction formula is as follows:

$$\left\{ \begin{array}{l} \hat{\lambda}_{new} \leftarrow \frac{\hat{\lambda}^2 + \epsilon^2}{2\epsilon} \quad |\lambda| < \epsilon \\ \epsilon_1 = 2.0 \max \left[0, (\lambda^R - \lambda^L) \right], \text{ or} \\ \epsilon_2 = 4.0 \max \left[0, (\hat{\lambda} - \lambda^L), (\lambda^R - \hat{\lambda}) \right]. \end{array} \right. \quad (4.11)$$

The formulation for the $\hat{\lambda}_{new}$ is exactly the same as Eqn. 4.7. However, a four times as wide a band as proposed by Harten and Hyman (1983) in formulation (2) is used for ϵ . This allows the expansion-shock to totally diffuse into the computational domain and completely disappear and a solution more consistent with the physical solution is obtained.

In formulation (4) either of ϵ_1 or ϵ_2 could be used for a wide range of test cases as given in this thesis without any re-tuning. The difference between the results obtained from ϵ_1 and ϵ_2 were not distinguishable for the test cases performed. However, ϵ_2 is selected here as it contains information from both sides of the cell face for which the entropy condition is enforced. In fact it can be shown that for the Burgers' equation ϵ_2 reduces to ϵ_1 .

Formulation (4) is applied to the scalar Burgers' equation and the result is shown in Fig. 4.2-f with a first order scheme. The same entropy fix formula, i.e. Formula (4), is applied to the shock tube problem and the result is shown in Fig. 4.4-f. As shown in Figs. 4.2-f and 4.4-f, Formula (4) has totally diffused the expansion shock and replaced it by an expansion fan in the sonic-expansion region. The proposed entropy fix formula, i.e. Formula (4), has been later extended to the second order Roe scheme, the results of which are shown in Figs. 4.2-f and 4.4-f for Burgers' equation and shock tube problem, respectively. For the second order scheme the MUSCL idea (due to van Leer (1979)) is used to extrapolate the primitive variables; pressure, velocity and either of temperature or density to the cell face. The unwanted numerical oscillations are damped with the minmod flux limiter (Tannehill et. al. (1997)). The method is later extended to 2-dimensional cases as explained below.

4.4 Inviscid Shear Flow

The system of Euler equations admits several kinds of discontinuities. Excluding shock waves, where all the primitive variables experience abrupt changes, other kinds of discontinuities also exist. Slip lines or shear flows are some examples, as explained here. Slip lines are defined by the condition of uniform pressure but an abrupt change of tangential velocity, as shown in Fig. 4.5. This problem is analyzed here.

Two parallel streams with the Mach numbers, $M_{in_A} = 2.00$ and $M_{in_B} = 4.00$ enter the domain of computation. According to the nature of inviscid flow governed by the Euler equations, there are no means by which the two streams could diffuse into one another. Therefore, the same condition as the inlet should be faithfully recovered all over the computational domain.

In this computation 91×81 uniform grids are used. As the solution advances, the inlet boundary condition dominates throughout the domain. This procedure is shown at the intermediate iteration numbers 400 and the final converged iteration number 4000, in Figs. 4.6 and 4.7, respectively. In these figures velocity vectors together with the iso-Mach lines are shown.

Fig. 4.8 shows the Mach number distribution across the computational domain at the locations $x = -0.3, 0.0, 0.3, 0.6, 0.9$. As shown in this figure, all of the predictions overlap each other and just one line is seen. The numerical algorithm used here, flux difference splitting (FDS) scheme of Roe (1981), is first order. However, the discontinuity is captured within only two grid points. The same problem has also been solved by Manna (1992) with similar results. This confirms that the numerical algorithm of Roe (1981) is non-diffusive and is very suitable for shear layers in compressible flows. For the same problem when the flux vector splitting (FVS) scheme of van Leer (1982) is used, the discontinuity is smeared over 6 grid points with a first order scheme. When a second order FVS of van Leer is applied the smearing reduces to 4. Manna's (1992) results are worse than the results of the first order prediction by the Roe scheme. With the same grid configuration when a central difference scheme is applied the smearing is even worse as compared to van Leer's.

The flow streams in this problem are along the grid. This is called *grid-aligned flow*. This makes the FDS scheme of Roe non-diffusive. However when the same flow is analyzed over a non-aligned grid, the degree to which the discontinuity smears over the grids depends on the flow angle with grid lines. However the smearing is much worse in the FVS of van Leer and even more so when any one of the central difference schemes is used. According to Manna, as indicated in the lecture notes for the von Karman Institute (1992), there is no scheme which can show better resolution than Roe's (1981) for this problem.

4.5 Transonic Channel Flow Over a Bump

This is a standard test case, as proposed by Rizzi and Viviani for a workshop in the *Notes on Numerical Fluid Mechanics* (1981). The transonic channel flow over a 4.2% thick bump at the bottom wall is studied here as depicted in Fig. 4.9. The thickness of the bump is 4.2% of the chord. The chord's leading edge is located at $x = -0.5$ and its trailing edge at $x = 0.5$. That is, the maximum thickness of the bump will be at $x = 0$. The inlet of the channel is located at $x = -2.0$ and the

exit plane at $x = 3.0$. The distance between the walls (except at the bump) is 2.073 times the chord length of the bump.

In our study according to Rizzi and Viviani (1981) the ratio of the static downstream pressure to upstream total pressure corresponds to $Mach = 0.85$.

For the subsonic channel flow over the bump, the flow accelerates as it passes the leading edge of the bump and approaches the maximum thickness of the bump. If the inflow Mach number, $Mach_{in}$, is less than a certain value, the so called *critical Mach number*, M_c , flow will be subsonic everywhere including over the bump. If $Mach_{in}$ increases and just reaches M_c a sonic spot over the bump appears, i.e. $Mach_{in} = M_c$. If $Mach_{in}$ continues to increase gradually, the spot will grow and a supersonic pocket will appear as sketched in Fig. 4.11. Therefore the transonic flow is called a *supercritical flow*. This flow in the pocket, which is supersonic, becomes subsonic flow via a normal shock located at x_{shock} , as shown in Fig. 4.11. The supersonic pocket is separated from the subsonic flow field by the sonic line, i.e. the locus of $M = 1$, as shown by a dashed line in Fig. 4.11. One end of the sonic line intersects the bump, say at x_{sonic} . The sonic line passes its maximum point, (x_{max}, y_{max}) , then connects to the normal shock at the end of supersonic pocket.

This case is solved numerically over a 91×41 grid, which is clustered near the bottom wall as shown in Fig. 4.10. The clustering allows better capture of the flow gradients close to the bottom wall. The clustering factor used here is 1.3.

The boundary conditions are as follows. In the subsonic inflow, stagnation pressure, stagnation temperature, and flow angle are specified. Also static pressure is extrapolated from interior domain to the inflow plane. In the subsonic outflow, static pressure is specified and the rest of flow parameters are extrapolated from the interior domain to the exit plane. At the surface of the wall, no-penetration through the solid wall is permitted ($\vec{V} \cdot \hat{n} = 0$, where $\vec{V}$ is the velocity vector and $\hat{n}$ is the unit vector normal to the wall). Surface pressure is determined from the momentum equation in the normal direction to the wall and the total temperature at the wall is set to that of the free stream as the steady inviscid flow is computed. Figure 4.12 shows the iso-Mach lines over the bump in channel flow in the transonic regime. Some iso-Mach lines are labeled in this figure including the sonic line, i.e.

$Mach = 1.00$. The region enclosed between the sonic line, the surface of the bump and the terminating normal shock is the supersonic pocket.

Figure 4.13 shows the *Mach* number distribution over the bottom and top walls. As shown in this figure the shock wave is very sharply captured. Also shown in this figure the *Mach* number profile at the inlet plane is uniform. However, at the exit plane there is an offset. This offset at the exit plane is due to two factors and is explained as follows: (1)- Flow stream lines at the bottom wall of the channel experience a shock wave over the bump. This reduces the stagnation pressure. Thus, with the uniform *Mach* number and stagnation pressure at the inlet, and with uniform back pressure specified at the exit plane, the *Mach* number at the bottom wall of the exit plane is smaller. (2)- Spurious entropy production is present at the grid discontinuities, Maarel and Koren (1990). This phenomena is more severe at the bottom wall where grid lines are skewed and the flow is not totally aligned with the grid and some unintentional numerical diffusion is introduced due to the presence of the bump. Therefore, the stagnation pressure is reduced. In a fully subsonic flow, i.e. with $Mach_{in} < M_c$, over the bump, the condition (1) does not apply but the condition (2) still persists and generates entropy which causes the *Mach* number at the bottom wall to be still smaller than that at the top wall at the exit plane. To reduce the phenomena of entropy generation as described in the condition (2) a smooth grid as much aligned with the flow is recommended. For this reason, quadrilateral grids which can better be aligned with the flow are more suitable for the flow computation because they can better be aligned with the flow as opposed to triangular grids. This matter is discussed in detail in the next chapter.

The physics of the flow over the bump has qualitatively been discussed above. Quantitative discussion and comparison for this test case is given here. Complete details of these computations would be very lengthy, therefore some key features and points are chosen for the comparison purposes. Among them are: the location of the normal shock, the geometry of the sonic line, e.g. the location that the sonic line intersects the bump and the maximum point of the sonic-line curve. Also in the computations of Manna (1992), *Mach* numbers upstream and downstream of the normal shock were reported which will also be compared. The details of all of

these four different computations together with the results obtained from the current computation are all assembled in Table 4.1, which shows a deviation of $\approx 2\%$.

4.6 De Laval Nozzle

Transonic flow in a converging-diverging nozzle also called a *De Laval nozzle* is the last test case studied here. The geometry of the nozzle is shown in Fig. 4.14 and its contour is defined by a third order polynomial on each side of the throat as follows:

Top:

$$y_{top} = \begin{cases} a_0 & -5.0 \leq x < \alpha, \\ b_0 + b_2x^2 + b_3x^3 & \alpha \leq x < 0, \\ c_0 + c_2x^2 + c_3x^3 & 0.0 \leq x < \beta, \\ d_0 & \beta \leq x \leq 8.5. \end{cases} \quad (4.12)$$

Bottom:

$$y_{bottom} = -y_{top}. \quad (4.13)$$

where

$$\begin{aligned} a_0 &= 1.00040 \\ b_0 &= 0.725, \quad b_2 = 0.0832, \quad b_3 = -0.0176016 \\ c_0 &= 0.725, \quad c_2 = 0.0208, \quad c_3 = -0.0022002 \\ d_0 &= 1.00034 \\ \alpha &= -3.15123, \quad \beta = 6.24877 \end{aligned}$$

For this test case, a 119×27 grid is taken as shown in Fig. 4.15. The boundary conditions are similar to that of a previous test case and are not repeated here.

Three different flow Mach numbers in the De Laval nozzle are studied, namely, $Mach_{in}=0.6$, 0.7 , and 0.8 . These flow Mach numbers are computed based on the ratio of the exit plane static pressure to the inlet plane stagnation pressure.

The results of the current study are shown Fig. 4.16. Mach number contours for the three flow speeds $Mach_{in} = 0.6$, 0.7 , and 0.8 are shown in Fig. 4.16-1, Fig. 4.16-2,

and Fig. 4.16-3, respectively. As shown in these figures, shock waves move toward downstream as the Mach number increases or in other words as the inflow stagnation pressure increases. The Mach number distribution along the center line for the three speeds is shown in Fig. 4.16-4, and static pressure distribution along the center is shown in Fig. 4.16-5. From Fig. 4.16-4 and Fig. 4.16-5, one can say that as the flow accelerates, the shock wave moves downstream.

Also from Fig. 4.16-4 and Fig. 4.16-5 it is clear that the shock wave has been captured very sharply. This is due the non-diffusive characteristic of the Roe scheme. With any other scheme such as Van Leer it was not possible to capture the shock within three nodes due to their diffusive behavior.

In the diverging portion of the nozzle, flow is supersonic upstream of the shock wave. This requires a choked flow at the throat of the nozzle, i.e. $Mach_{throat} = 1$. That is, a sonic expansion is performed at the throat of the nozzle and the Roe scheme supposedly performs non-physical behavior. In this acceleration process, the expansion shock is avoided at the throat by applying the current entropy correction formula, i.e. formula (4).

The results of the current study for all of the three speeds is compared with the analytical results of a quasi one-dimensional flow which are summarized in Table 4.2.

For the given back pressure, the location of the shock wave could also be determined for comparison purposes. This is a time consuming iterative procedure. Rather, the location of the shock could be taken from the current study and then the exit pressure and *Mach* number to be determined by the analytical results of a quasi one-dimensional flow. This task has been performed and the results are summarized in the Table 4.3 for comparison.

The comparison between the current study and the analytical results of a quasi one-dimensional flow show average differences of 1 % or less.

4.7 Conclusion

A simple modification is applied to the Harten-Hyman entropy fix formulation and the new entropy fix formula is applied to several test cases. The proposed formula

can totally diffuse the expansion shocks in sonic-expansion regions. It showed a robust behavior, since it needed no re-tuning for the wide range of applications from the scalar Burgers' equation to multi-dimensional flows.

Table 4.1: Transonic flow comparison over a bump.

Computed by.	x_{sonic}	x_{shock}	x_{max}	y_{max}	M_x	M_y	M_{y*}^a	%Error M_y
Current computation	-0.18	0.31	0.16	0.79	1.26	0.822	0.807	1.86%
Veulliot & Viviand ^b	-0.19	0.33	0.20	0.82	N/A	N/A	N/A	N/A
Deconinck & Hirsch ^c	-0.2	0.31	0.17	0.69	N/A	N/A	N/A	N/A
Lerat & Sides ^d	-0.18	0.31	0.16	0.80	N/A	N/A	N/A	N/A
Manna (1992)	N/A	N/A	N/A	N/A	1.31	0.77	0.781	1.43%

^a M_{y*} is determined from the normal shock relations, Rankine-Hugoniot, corresponding to M_x .

^bSee Reference: Rizzi and Viviand (1981)

^cSee Reference: Rizzi and Viviand (1981)

^dSee Reference: Rizzi and Viviand (1981)

Table 4.2: Transonic flow comparison in a converging-diverging nozzle (De Laval Nozzle).

Case	M_x^a	M_y^b	$(M_y)_{theory}^c$	$\frac{p_y}{p_x}^d$	$(\frac{p_y}{p_x})_{theory}^e$	Average Error
1	1.426	0.7212	0.7290	2.211	2.206	1.07 %
2	1.585	0.6667	0.6730	2.769	2.764	Less than 1 %
3	1.712	0.6371	0.6375	3.246	3.253	Less than 1 %

^aMach number at upstream of the shock at the center line by current computation.

^bMach number at downstream of the shock at the center line by current computation.

^cMach number downstream of the normal shock obtained from the Rankine-Hugoniot relation with M_x given.

^dpressure ratio across the shock by current computation.

^epressure ratio across the shock obtained from the Rankine-Hugoniot.

Table 4.3: Comparison of the Mach number and pressure at the center line of the exit plane of the De Laval Nozzle.

Case	M_e^a	$(M_e)_{theory}^b$	p_e^c	$(p_e)_{theory}^d$	Average Error
1	0.5209	0.51724	101300	102114	Less than 1 %
2	0.5616	0.5608	101300	101970	Less than 1 %
3	0.6095	0.6115	101300	102203	Less than 1 %

^aexit *Mach* number obtained from the current computation.

^bexit *Mach* number obtained from analytical results of a quasi one-dimensional flow.

^cexit pressure obtained from the current computation.

^dexit pressure obtained from analytical results of a quasi one-dimensional flow.

Figure 4.1: Initial condition for the Burgers' equation.

Figure 4.2: Solution of the Burgers' equation at time $t = 1$ sec.

Figure 4.3: Schematic of shock tube problem, (a)- initial condition, (b)- sometime after the diaphragm is broken.

Figure 4.4: Solution of the shock tube problem at time $t = 3.9$ milli sec.

Figure 4.5: Schematic picture of inviscid shear flow (slipline).

Figure 4.6: Inviscid shear flow with iso-Mach lines at iteration =400.

Figure 4.7: Final converged solution for the inviscid shear flow.

Figure 4.8: Mach number distribution along the transverse direction at $x = -0.3, 0.0, 0.3, 0.6, 0.9$. All the profiles overlapped on a single profile.

Figure 4.9: Schematic shape of the channel flow with 4.2% bump.

Figure 4.10: Grid configuration for the flow over the bump; 91×41 grid with a clustering factor 1.3 at the bottom wall.

Figure 4.11: Schematic of supercritical flow over a bump for a supercritical flow.

Figure 4.12: Iso-Mach lines over the bump in a transonic flow with supersonic pocket.

Figure 4.13: Mach distribution along the top and bottom walls of transonic channel flow.

Figure 4.14: The configuration of *De Laval Nozzle* applied to transonic flow.

Figure 4.15: Grid configuration for the De Laval Nozzle: 119×27 .

Figure 4.16: De Laval Nozzle computations by the current study, (1) to (3) Iso Mach lines, (4) Mach number distribution along the center line, (5) Pressure distribution along the center line.

Chapter 5

Roe Scheme in Generalized Coordinates; Formulations

5.1 Introduction

The most important characteristic of the Roe scheme is that it is a fairly non-diffusive scheme in essence and the diffusive behavior that this scheme could show, is mostly due to the grid obliqueness w.r.t the flow. Solving a problem with the Roe scheme over two types of grids, one totally aligned with the flow and the other being oblique w.r.t the flow could elaborate on this matter. Consider an inviscid shear flow with two parallel streams with Mach numbers 2 and 4 as depicted in Fig. 5.1. Because these streams are assumed to be inviscid, there IS no mechanism by which one of the streams could diffuse into the other. Therefore, the same condition as at the inlet plane should continue through the whole domain. The first order accurate scheme of Roe captures this discontinuity within two grids, like the exact solution, as shown in Fig. 5.2. This is because the Roe scheme as an Approximate Riemann Solver (ARS), solves the approximate Riemann problem (the linearized problem) by exact method. When the same flow is analyzed with an oblique grid, the discontinuity smears over the grid with smearing depending on the flow angle with the grid, see Chapter 4 and Manna (1992) for more detail.

To more efficiently use the non-diffusive property of the Roe scheme, it is always

desired to align the grid with the flow as much as it is possible, although, to totally align the flow with the grid is usually a non-feasible task depending on the complexity of the geometry and the flow. However, the type of grid chosen for a problem could help to achieve this goal. For 2-dimensional cases with triangular grid shapes, in general, the grids can almost never be aligned with the flow to any degree. Therefore, the non-diffusive behavior of the Roe scheme, the characteristic for which it was originally developed, is partially lost. This is illustrated in Fig. 5.3, in which a triangular grid is compared with a quadrilateral H shaped grid in terms of the grid obliqueness with the flow. Near the solid walls, flow is almost aligned with the walls, therefore, the flow direction is somehow known to some extent in these regions. As shown in this figure, in general, the flow can be better aligned with quadrilateral H grids near the solid walls.

To solve the fluid equations by the Roe scheme over an H grid, there are two major approaches (as with any other scheme): (1)- to directly solve the equations on the physical domain, or (2)- to transform the fluid equations into generalized coordinates, then solve the equations in the computational domain. Most of the approaches to solve the fluid equations in the literature, use the first approach (Mazaheri and Abbasian (1998), Currie (1998), Frink et. al. (1991) and Hirsch (1990)). There are only a few reports available in the literature that address the second approach, and most of them are quite brief (see Tannehill et. al. (1997) and CFL3D Manual edited by Biedron and Rumsey (1998)). With the choice of quadrilateral grids, like H shaped grids, approach (1) offers no advantage over approach (2). Therefore, there is a need to clearly and explicitly address the solution of the fluid equations by the Roe scheme in generalized coordinates.

This chapter is split into two parts, (1) grid related materials concerned with one to one mapping between the physical and computational domain and (2) materials related to the discretization of fluid equations by the Roe scheme in generalized coordinates. Part (1) is general and could be used for any type of numerical scheme as applied on generalized coordinates. However part (2) is mainly devoted to the formulation of the Roe scheme in generalized coordinates.

There is a solid link between these two parts, because a comprehensive knowledge

of the grid is needed by the solver. Part (1) as mentioned above, is subdivided into the following sections: (i) the metrics of transformation that relate the physical- and computational domain to each other, (ii) the skewness (or cosine directions) of the grid lines and the control volume faces in terms of the metrics of transformation and (iii) the area of the cell faces again obtained in terms of the metrics of transformation. The sub-divisions (i), (ii) and (iii) are referred to as *grid-geometry* in this chapter.

In the discretization of fluid equations by the Roe scheme, i.e. part (2), the following materials are addressed: (i) the fluid equations in both the physical and computational domain are written and put side by side, term by term to obtain the relationship between their terms, (ii) the total mass, momentum and energy crossing each face of control volume in the physical domain is obtained by the relation (total mass=mass flux $\times$ cell face area, etc.) and it is shown that they are equal to the total mass, momentum and energy crossing the corresponding cell face in the computational domain, and (iii) the numerical flux based on the Roe scheme in generalized coordinates is obtained.

The application of the numerical flux based on the Roe scheme (obtained in this chapter) to inviscid and viscous flows are given in Chapter 6 and in Ref. [6].

5.2 Grid Geometry

To solve the governing equation of fluid motion, a comprehensive knowledge of the grid system is required by the flow solver. One way to detail and to make known the configuration of the grid system to the flow solver is through the metrics of transformation from the physical domain to the computational domain. In this approach, the following materials are determined: the normal direction to grid lines to each cell face, and the area of the cell faces that the fluxes cross. This knowledge is referred to as *grid-geometry* in this chapter. The grid-geometry in terms of the metrics of transformation are determined as follows.

5.2.1 Metrics of Transformation

Consider Fig. 5.4 in which the grid configuration in both the physical and the computational domain are shown. In the transformation from the physical domain to the computational domain, a one to one transformation is assumed. That is, a point in the physical domain, say point A , corresponds to one and only one point in the computational domain, point B , and vice versa. Therefore, a point in the physical domain and its correspondent in the computational domain could be denoted by the same index (j, k) . In general, the physical domain and the computational domain are related by:

$$x = x(\xi, \eta) \quad y = y(\xi, \eta) \quad (5.1)$$

This relationship could be determined in several ways, (1) algebraically, (2) by solving elliptic, hyperbolic or parabolic PDE's, or (3) by a given set of data. For any of the above-cases (1), (2) or (3) relation 5.1 applies and must somehow be introduced to the solver.

The metrics of transformation ξ_x , ξ_y , η_x , and η_y are the parameters that relate two domains in the following form, see for example Hoffmann and Chiang (1993).

$$\begin{aligned} \xi_x &= J \, y_\eta, \\ \xi_y &= -J \, x_\eta, \\ \eta_x &= -J \, y_\xi, \\ \eta_y &= J \, x_\xi, \end{aligned} \quad (5.2)$$

where J is the ratio of the volumes in the computational domain to that of the physical domain also called the *Jacobian of transformation*:

$$J = \frac{1}{x_\xi y_\eta - x_\eta y_\xi}, \quad (5.3)$$

and x_ξ , y_η , x_η , and y_ξ are the inverse metrics of transformation which are computed by central differencing for internal nodes, and one-sided differencing for the boundaries. The central difference form would be as follows.

$$x_\xi = \frac{x_{j+1,k} - x_{j-1,k}}{2\Delta\xi},$$

$$\begin{aligned}
y_\xi &= \frac{y_{j+1,k} - y_{j-1,k}}{2\Delta\xi}, \\
x_\eta &= \frac{x_{j,k+1} - x_{j,k-1}}{2\Delta\eta}, \\
y_\eta &= \frac{y_{j,k+1} - y_{j,k-1}}{2\Delta\eta}.
\end{aligned} \tag{5.4}$$

5.2.2 Cosine Directions of the Grid Lines

Fig. 5.5 shows a body fitted grid system, in which the body is denoted by a constant η line, say $\eta = 0$. The next line almost parallel to the body is denoted by $\eta = 1$ (assuming $\Delta\eta = 1$), and the following lines $\eta = 2, 3$, etc. The grid lines in the transverse direction are denoted by constant ξ lines.

The gradient of ξ , $\vec{\nabla}\xi$, is a vector pointing the direction of maximum change of ξ and it is normal to iso- ξ lines. The cosine direction of the unit vector $\hat{n}_\xi$ is along $\vec{\nabla}\xi$ and could be determined as follows:

$$\hat{n}_\xi \equiv \frac{\vec{\nabla}\xi}{|\vec{\nabla}\xi|} = \cos \theta \hat{i} + \sin \theta \hat{j}, \tag{5.5}$$

where θ is the angle between the vector $\vec{\nabla}\xi$ and the x -axis, $\vec{\nabla}\xi \equiv \xi_x \hat{i} + \xi_y \hat{j}$, and $|\vec{\nabla}\xi| = \sqrt{\xi_x^2 + \xi_y^2}$. This concludes:

$$\cos \theta = \frac{\xi_x}{\sqrt{\xi_x^2 + \xi_y^2}}, \quad \sin \theta = \frac{\xi_y}{\sqrt{\xi_x^2 + \xi_y^2}}. \tag{5.6}$$

Eqn. 5.6 shows the skewness of iso- ξ lines and will be used throughout this thesis.

Likewise, the normal direction to iso- η lines are determined from $\vec{\nabla}\eta$, where $\vec{\nabla}\eta$ is a vector showing the direction of maximum change in η . Therefore,

$$\hat{n}_\eta \equiv \frac{\vec{\nabla}\eta}{|\vec{\nabla}\eta|} = \cos \beta \hat{i} + \sin \beta \hat{j}, \tag{5.7}$$

where β is the angle between the vector $\vec{\nabla}\eta$ and x -axis, $\vec{\nabla}\eta \equiv \eta_x \hat{i} + \eta_y \hat{j}$, $|\vec{\nabla}\eta| = \sqrt{\eta_x^2 + \eta_y^2}$, and:

$$\cos \beta = \frac{\eta_x}{\sqrt{\eta_x^2 + \eta_y^2}}, \quad \sin \beta = \frac{\eta_y}{\sqrt{\eta_x^2 + \eta_y^2}}. \tag{5.8}$$

It should be noted that the formulations given here are not limited to orthogonal grids and also applies to non-orthogonal grids.

5.2.3 Cosine Directions at the Cell Faces

In the current study, all the information including those of the grid geometry and flow parameters are all stored at nodes. In fact this approach is called the *cell vertex* approach. Assuming the cell faces are located at the mid-point between the adjacent nodes, a simple interpolation can provide the grid geometry at the cell face. Fig. 5.6 shows the enlargement of the control volumes associated with node A (in physical-domain) and B (in computational-domain). The boundary of this control volume is represented by dashed lines and denoted by E (east), W (west), N (north), and S (south). Consider the unit vector normal to the face E . Its cosine directions are:

$$\hat{n}_{\xi_E} = \cos \theta_E \hat{i} + \sin \theta_E \hat{j} \quad (5.9)$$

where θ_E is the angle between the normal direction to the face E and the x-axis. Different types of interpolation could be used to obtain the cosine direction at the mid point E . The following arithmetic averaging is used in this thesis:

$$\begin{aligned} \cos \theta_E &\approx \frac{1}{2} [\cos \theta_{j+1,k} + \cos \theta_{j,k}] = \frac{1}{2} \left[\left(\frac{\xi_x}{\sqrt{\xi_x^2 + \xi_y^2}} \right)_{j+1,k} + \left(\frac{\xi_x}{\sqrt{\xi_x^2 + \xi_y^2}} \right)_{j,k} \right] \\ &= \left(\frac{\xi_x}{\sqrt{\xi_x^2 + \xi_y^2}} \right)_E \end{aligned} \quad (5.10)$$

and

$$\begin{aligned} \sin \theta_E &\approx \frac{1}{2} [\sin \theta_{j+1,k} + \sin \theta_{j,k}] = \frac{1}{2} \left[\left(\frac{\xi_y}{\sqrt{\xi_x^2 + \xi_y^2}} \right)_{j+1,k} + \left(\frac{\xi_y}{\sqrt{\xi_x^2 + \xi_y^2}} \right)_{j,k} \right] \\ &= \left(\frac{\xi_y}{\sqrt{\xi_x^2 + \xi_y^2}} \right)_E. \end{aligned} \quad (5.11)$$

Similarly at the north boundary of this control volume, i.e. at face N of the control volume:

$$\hat{n}_{\eta_N} = \cos \beta_N \hat{i} + \sin \beta_N \hat{j} \quad (5.12)$$

where:

$$\begin{aligned} \cos \beta_N &\approx \frac{1}{2} [\cos \beta_{j,k+1} + \cos \beta_{j,k}] = \frac{1}{2} \left[\left(\frac{\eta_x}{\sqrt{\eta_x^2 + \eta_y^2}} \right)_{j,k+1} + \left(\frac{\eta_x}{\sqrt{\eta_x^2 + \eta_y^2}} \right)_{j,k} \right] \\ &= \left(\frac{\eta_x}{\sqrt{\eta_x^2 + \eta_y^2}} \right)_N \end{aligned} \quad (5.13)$$

and

$$\begin{aligned}\sin \beta_N &\approx \frac{1}{2} [\sin \beta_{j,k+1} + \sin \beta_{j,k}] = \frac{1}{2} \left[\left(\frac{\eta_y}{\sqrt{\eta_x^2 + \eta_y^2}} \right)_{j,k+1} + \left(\frac{\eta_y}{\sqrt{\eta_x^2 + \eta_y^2}} \right)_{j,k} \right] \\ &= \left(\frac{\eta_y}{\sqrt{\eta_x^2 + \eta_y^2}} \right)_N.\end{aligned}\quad (5.14)$$

Eqns. 5.10 and 5.13 give the cosine directions and Eqns. 5.11 and 5.14 give the sine directions of the control volume faces as function of the metrics of transformation in a clear and explicit form (the angle between control volume faces and positive x-axis). To the best knowledge of the author, no such relations have been given before in this clear and explicit form, in order to obtain the skewness of the cell faces.

5.2.4 Area of the Cell Faces

The boundaries of the control volume A consist of area segments ΔS_E , ΔS_N , etc. To obtain total mass (total mass=mass-flux $\times$ area), momentum and energy passing through these area's, we need to obtain the magnitude of these area's. Consider cell-face E with the area ΔS_E . Its projected area along the x and y axes are $(-\Delta x)$ and Δy , respectively. Therefore,

$$\Delta S_E^2 = (-\Delta x)^2 + (\Delta y)^2. \quad (5.15)$$

Noting that ΔS_E (from the physical domain) corresponds to $\Delta \eta$ (from the computational domain). Hence,

$$\Delta S_E^2 = \left[\left(\frac{\Delta x}{\Delta \eta} \right)^2 + \left(\frac{\Delta y}{\Delta \eta} \right)^2 \right] (\Delta \eta)^2, \quad (5.16)$$

or

$$\Delta S_E^2 = [x_\eta^2 + y_\eta^2] (\Delta \eta)^2, \quad (5.17)$$

and applying Eqns. 5.2 we obtain:

$$\Delta S_E = \left[\frac{\sqrt{\xi_x^2 + \xi_y^2}}{J} \right]_E \Delta \eta. \quad (5.18)$$

A similar equation for the cell face area of the north boundary, ΔS_N , is obtained as follows:

$$\Delta S_N = \left[\frac{\sqrt{\eta_x^2 + \eta_y^2}}{J} \right]_N \Delta \xi. \quad (5.19)$$

Eqns. 5.18 and 5.19 are very serviceable and beneficial equations, which give the area of the control volume faces in terms of the metrics of transformation. Eqns. 5.18 and 5.19 relate the area of the control volumes in the physical domain (ΔS_E or ΔS_N etc.) to the area of the control volume in the computational domain ($\Delta \eta$ or $\Delta \xi$). To the best knowledge of the author, no such relations have been given before, in this clear and explicit form, in order to obtain the area of the control volume faces as functions of the metrics of transformation. These equations will be used throughout this thesis to compute the area of control volume faces.

At this point a comprehensive knowledge of the grid-geometry is obtained. That is, the angle of control volume faces with positive x-axis and the area of the control volume faces are obtained, as functions of metrics of transformation. For the rest of this chapter the fluid equations will be discretized in order to give the numerical flux based on the Roe scheme in generalized coordinates.

5.3 Fluid Equations in the Physical Domain

The inviscid compressible flow equations in full conservative form with no body force, as written in Chapter 3, is repeated here for convenience:

$$\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0 \quad (5.20)$$

where Q , F , and G are:

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ E_t \end{bmatrix}, \quad F = \begin{bmatrix} \rho u \\ p + \rho u^2 \\ \rho uv \\ (E_t + p)u \end{bmatrix}, \quad G = \begin{bmatrix} \rho v \\ \rho uv \\ p + \rho v^2 \\ (E_t + p)v \end{bmatrix}, \quad (5.21)$$

where ρ , p , u , v , E_t are density, pressure, x- and y- velocity component, and the total energy per unit volume, respectively. E_t is the sum of the internal- and kinetic-energy per unit volume given by: $E_t = \rho(e + \frac{V^2}{2})$, where $V^2 = u^2 + v^2$ and e is the

internal energy per unit mass. For a calorically perfect gas, pressure is estimated by the equation of state: $p = \rho(\gamma - 1)e$, where γ is the ratio of specific heats, which is constant for perfect gases with a value of 1.4 when applied to air. Eqn. 5.20 could be written in a compact form as follows:

$$\frac{\partial Q}{\partial t} + \vec{\nabla} \cdot \vec{R} = 0 \quad (5.22)$$

where $\vec{R}$ is the total flux vector, given by $\vec{R} = F \hat{i} + G \hat{j}$ and $\hat{i}$ and $\hat{j}$ are the unit vectors along the x and y axes, respectively.

Integrating Eqn. 5.22 over an arbitrary volume V gives:

$$\int_V \frac{\partial Q}{\partial t} dV + \int_V \vec{\nabla} \cdot \vec{R} dV = 0. \quad (5.23)$$

Considering the first integral of Eqn. 5.23 and assuming any kind of arbitrary variations for Q over V , see Fig. 5.7, an average $\bar{Q}$ could be defined as follows:

$$\bar{Q} \equiv \frac{1}{V} \int_V Q dV. \quad (5.24)$$

The second term in Eqn. 5.23, is a volume integral over V , which is converted to a surface integral through the Divergence (Gauss) theorem, i.e. $\int_V \vec{\nabla} \cdot \vec{R} dV \equiv \oint_S \vec{R} \cdot d\vec{S}$, where S is the surface surrounding V and $d\vec{S}$ is the surface element vector, which is normal to the surface and aims outward, as shown in Fig. 5.7. Hence Eqn. 5.23 becomes:

$$V \frac{\partial \bar{Q}}{\partial t} + \oint_S \vec{R} \cdot d\vec{S} = 0 \quad (5.25)$$

Eqn. 5.25 is the integral form of the fluid equation, Eqn. 5.20. Eqn. 5.25 represents the rate of change of the mean value of Q over the control volume V (see Fig. 5.7), which varies by the net flux $\vec{R}$ crossing the closed surface S . Eqn. 5.25 is expanded over the control volume A of Fig. 5.6:

$$V \frac{\partial \bar{Q}}{\partial t} + R_{E_n} \Delta S_E + R_{N_n} \Delta S_N - R_{W_n} \Delta S_W - R_{S_n} \Delta S_S = 0, \quad (5.26)$$

where R_{E_n} , R_{N_n} , etc. are the numerical fluxes normal to the cell faces and they are in the physical domain and must be determined. In Eqn. 5.26, it should be noted that $(\vec{R} \cdot d\vec{S})_E = R_{E_n} \Delta S_E$ because the normal component of $\vec{R}_E$ is taken to be

in the same direction as $d\vec{S}_E$, so the dot product is positive. On the other hand, $(\vec{R} \cdot d\vec{S})_W = -R_{W_n} \Delta S_W$ because the normal component of $\vec{R}_W$ is in the opposite direction of $d\vec{S}_W$, so the dot product is negative.

5.4 Fluid Equations in Generalized Coordinates

Eqn. 5.20 is transformed to a generalized coordinate system by the chain rule,

$$\begin{aligned}\frac{\partial}{\partial t} &= \frac{\partial}{\partial \tau}, \\ \frac{\partial}{\partial x} &= \xi_x \frac{\partial}{\partial \xi} + \eta_x \frac{\partial}{\partial \eta}, \\ \frac{\partial}{\partial y} &= \xi_y \frac{\partial}{\partial \xi} + \eta_y \frac{\partial}{\partial \eta}\end{aligned}\tag{5.27}$$

Viviand (1974) and Vinokur (1974) separately have shown that the resulting equations can be written in a strong conservation form similar to the original equations in the physical domain. This allows that all the shock capturing techniques as applied to fluid equations in the physical domain can be applied to the fluid equations in generalized coordinates as well. This is because this type of equation does not change in the transformation. For example, if the original equation in the physical domain is hyperbolic, it will remain hyperbolic in any other coordinate system.

The fluid equations for the inviscid, unsteady and compressible flow in full conservative form in generalized coordinates becomes:

$$\frac{\partial Q_1}{\partial t} + \frac{\partial F_1}{\partial \xi} + \frac{\partial G_1}{\partial \eta} = 0\tag{5.28}$$

where

$$Q_1 \equiv \frac{Q}{J}, \quad F_1 \equiv \frac{1}{J} (\xi_x F + \xi_y G), \quad G_1 \equiv \frac{1}{J} (\eta_x F + \eta_y G).\tag{5.29}$$

Eqn. 5.28 is integrated over the control volume B , shown in Fig. 5.6. Note that the control volumes A and B are equivalent maps of each other; the first one in the physical domain, and the second one in the computational domain. That is each point of the control volume A corresponds to only one point of control volume B and vice versa. Also each face of A , say face E , corresponds to the same face, face E ,

of control volume B . Integrating Eqn. 5.28 over B and applying the Gauss theorem gives:

$$(Vol.)_{comp.} \frac{\partial \bar{Q}_1}{\partial t} + F_{1E} \Delta \eta + G_{1N} \Delta \xi - F_{1W} \Delta \eta - G_{1S} \Delta \xi = 0, \quad (5.30)$$

where $(Vol.)_{comp.} = \Delta \xi \Delta \eta \times 1$, and F_{1E} , G_{1N} , etc. are the numerical fluxes in the computational domain.

5.5 Relating Equations of the Physical- and Computational-Domain

After writing the fluid equations in both of the physical domain or Cartesian coordinates (Eqn. 5.26) and the computational domain or generalized coordinates (Eqn. 5.30), the relation between the terms of these equations are addressed by putting side by side the terms of these equations.

First term: The volume of the control volumes A and B are related by the Jacobian of transformation, i.e.

$$J \equiv \frac{(Vol.)_{comp.}}{(Vol.)_{phy.}} = \frac{\Delta \xi \Delta \eta}{V}. \quad (5.31)$$

On the other hand according to Eqn. 5.29, one can write: $\bar{Q}_1 = \bar{Q}/J$. Therefore, the first term of Eqn. 5.30 becomes:

$$(Vol.)_{comp.} \frac{\partial \bar{Q}_1}{\partial t} = \frac{(Vol.)_{comp.}}{J} \frac{\partial \bar{Q}}{\partial t} = V \frac{\partial \bar{Q}}{\partial t}, \quad (5.32)$$

which is exactly the same as the first term of Eqn. 5.26.

The other terms: Similarly, it can be shown that the other terms of Eqns. 5.26 and 5.30 are equivalent. This task is performed for the second term of the Eqns. 5.26 and 5.30, i.e. for the terms corresponding to the cell face E .

Face E of the control volume A has an area of ΔS_E . Assuming all the flow parameters are known at this face, the flux vectors F and G can be determined from Eqn. 5.21 and the total flux vector, $\vec{R}$, at this cell face could be written as:

$$\vec{R}_E \equiv F_E \hat{i} + G_E \hat{j}. \quad (5.33)$$

The schematic picture of $\vec{R}_E$ and its components, F_E and G_E , are shown in Fig. 5.8.

$$\vec{R}_E = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uH \end{bmatrix}_E \hat{i} + \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vH \end{bmatrix}_E \hat{j}. \quad (5.34)$$

After combining terms F_E and G_E :

$$\vec{R}_E = \begin{bmatrix} \rho(u\hat{i} + v\hat{j}) \\ \rho u(u\hat{i} + v\hat{j}) + p\hat{i} \\ \rho v(u\hat{i} + v\hat{j}) + p\hat{j} \\ \rho H(u\hat{i} + v\hat{j}) \end{bmatrix}_E, \quad (5.35)$$

$u_E \hat{i} + v_E \hat{j}$ is the total velocity at the cell face E and is denoted by $\vec{V}_E$. The velocity vector $\vec{V}_E$ and its components are shown in Fig. 5.9. Therefore, Eqn. 5.35 can be written in the compact form of:

$$\vec{R}_E = \begin{bmatrix} \rho \vec{V} \\ \rho u \vec{V} + p\hat{i} \\ \rho v \vec{V} + p\hat{j} \\ \rho H \vec{V} \end{bmatrix}_E. \quad (5.36)$$

The surface area ΔS_E is a vector normal to ΔS_E aiming outward, as shown in Fig. 5.10. The component of $\vec{R}_E$ along $\Delta \vec{S}_E$ is called R_{E_n} . R_{E_n} is determined by forming the dot product between the vectors $\vec{R}_E$ and the unit vector $\hat{n}_E$ (the unit vector along $\Delta \vec{S}_E$, see Fig. 5.10), i.e.

$$R_{E_n} \equiv \vec{R}_E \cdot \hat{n}_E = \begin{bmatrix} \rho \vec{V} \\ \rho u \vec{V} + p\hat{i} \\ \rho v \vec{V} + p\hat{j} \\ \rho H \vec{V} \end{bmatrix}_E \cdot \hat{n}_E \quad (5.37)$$

and

$$\hat{n}_E = \cos \theta_E \hat{i} + \sin \theta_E \hat{j}. \quad (5.38)$$

The component of $\vec{V}_E$ along $\Delta\vec{S}_E$ is denoted by $u_{\perp E}$ as depicted in Fig. 5.11. $u_{\perp E}$ is determined by:

$$u_{\perp E} \equiv \vec{V}_E \cdot \hat{n}_E = u_E \cos \theta_E + v_E \sin \theta_E. \quad (5.39)$$

From Eqns. 5.10 and 5.11, $\cos \theta_E$ and $\sin \theta_E$ can be substituted for in Eqn. 5.39. It results in:

$$u_{\perp E} = \left[u \frac{\xi_x}{\sqrt{\xi_x^2 + \xi_y^2}} + v \frac{\xi_y}{\sqrt{\xi_x^2 + \xi_y^2}} \right]_E. \quad (5.40)$$

On the other hand, $\hat{i} \cdot \hat{n}_E$ is the component of $\hat{n}_E$ along the x-axis, i.e. $\cos \theta_E$. Similarly, $\hat{j} \cdot \hat{n}_E = \sin \theta_E$. Hence Eqn. 5.37 becomes:

$$R_{E_n} = \begin{bmatrix} \rho u_{\perp} \\ \rho u u_{\perp} + p \cos \theta \\ \rho v u_{\perp} + p \sin \theta \\ \rho u_{\perp} H \end{bmatrix}_E, \quad (5.41)$$

This is the normal components of the total flux at face E . Total mass (mass flux $\times$ area), momentum and energy crossing this face are represented by $R_{E_n} \Delta S_E$ and are determined as follows (ΔS_E is taken from Eqn. 5.18):

$$R_{E_n} \Delta S_E = \begin{bmatrix} \rho \left(u \frac{\xi_x}{\sqrt{\xi_x^2 + \xi_y^2}} + v \frac{\xi_y}{\sqrt{\xi_x^2 + \xi_y^2}} \right) \\ \rho u \left(u \frac{\xi_x}{\sqrt{\xi_x^2 + \xi_y^2}} + v \frac{\xi_y}{\sqrt{\xi_x^2 + \xi_y^2}} \right) + p \frac{\xi_x}{\sqrt{\xi_x^2 + \xi_y^2}} \\ \rho v \left(u \frac{\xi_x}{\sqrt{\xi_x^2 + \xi_y^2}} + v \frac{\xi_y}{\sqrt{\xi_x^2 + \xi_y^2}} \right) + p \frac{\xi_y}{\sqrt{\xi_x^2 + \xi_y^2}} \\ \rho \left(u \frac{\xi_x}{\sqrt{\xi_x^2 + \xi_y^2}} + v \frac{\xi_y}{\sqrt{\xi_x^2 + \xi_y^2}} \right) H \end{bmatrix}_E \underbrace{\left(\frac{\sqrt{\xi_x^2 + \xi_y^2}}{J} \right)_E \Delta \eta}_{\Delta S_E}. \quad (5.42)$$

Eqn. 5.42 is simplified as follows:

$$R_{E_n} \Delta S_E = \begin{bmatrix} \rho \left(u \frac{\xi_x}{J} + v \frac{\xi_y}{J} \right) \\ \rho u \left(u \frac{\xi_x}{J} + v \frac{\xi_y}{J} \right) + p \frac{\xi_x}{J} \\ \rho v \left(u \frac{\xi_x}{J} + v \frac{\xi_y}{J} \right) + p \frac{\xi_y}{J} \\ \rho \left(u \frac{\xi_x}{J} + v \frac{\xi_y}{J} \right) H \end{bmatrix}_E \Delta \eta. \quad (5.43)$$

Eqn. 5.43 could be split into two terms as:

$$R_{E_n} \Delta S_E = \left(\frac{\xi_x}{J} \right)_E \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uH \end{bmatrix}_E \Delta \eta + \left(\frac{\xi_y}{J} \right)_E \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vH \end{bmatrix}_E \Delta \eta. \quad (5.44)$$

According to Eqn. 5.21:

$$R_{E_n} \Delta S_E = \left[\left(\frac{\xi_x}{J} \right) F + \left(\frac{\xi_y}{J} \right) G \right]_E \Delta \eta. \quad (5.45)$$

Finally according to Eqn. 5.29:

$$R_{E_n} \Delta S_E = F_{1_E} \Delta \eta. \quad (5.46)$$

Eqn. 5.46 is a very meaningful equation for variety of reasons as described below:

1. $R_{E_n} \Delta S_E = F_{1_E} \Delta \eta$ represents the total mass (=mass flux $\times$ area), momentum and energy crossing the cell face E in the physical domain, which are in turn equivalent to that crossing the corresponding face E in the computational domain. This is explained as follows. In Eqn. 5.46, R_{E_n} represents the numerical flux of mass, momentum and energy crossing the cell face E in the physical domain. When R_{E_n} is multiplied by its corresponding area (ΔS_E), it gives the total mass (total mass=mass-flux $\times$ area), momentum and energy crossing the face E in the physical domain. On the other hand, F_{1_E} is the numerical flux crossing face E in the computational domain and $F_{1_E} \Delta \eta$ represents the total mass, momentum and energy crossing the face E in the computational domain. Eqn. 5.46 explicitly demonstrates that the total mass, momentum and energy crossing the face E in both of the domains are same.
2. Secondly, it shows that the second terms of Eqns. 5.26 and 5.30 are identical. This allows the same idea to be extended to the other terms of Eqns. 5.26 and 5.30 as well.

5.6 Numerical Flux Based on the Roe Scheme in Physical Domain

To obtain an appropriate form for the numerical flux based on the Roe scheme in the computational domain (generalized coordinates), it is assumed that the numerical flux based on the Roe scheme in the physical domain is given (see Appendix D-Eqn. D.13) and its numerical flux in generalized coordinates is obtained.

Again it is started with the face E :

$$R_{E_n} = \frac{1}{2} [R_{E_n}^L + R_{E_n}^R] - \frac{1}{2} \sum_{\kappa=1}^4 |\hat{\lambda}_E^{(\kappa)}| \delta w_E^{(\kappa)} \hat{T}_E^{(\kappa)}, \quad (5.47)$$

where $R_{E_n}^L$ and $R_{E_n}^R$ are the normal components of the total fluxes at face E obtained at inner (L) and outer (R) conditions (see Fig. 5.12), $\hat{\lambda}_E$'s are the eigenvalues of the Jacobian matrix determined at Roe's averaged condition, δw_E 's are the wave amplitudes and $\hat{T}_E$'s are the eigenvectors corresponding to the eigenvalues ($\hat{\lambda}_E$'s) determined at Roe's averaged conditions. The term R_{E_n} on the L.H.S. of Eqn. 5.47 is the numerical flux, based on the Roe scheme (total-mass, momentum, or energy per unit area of the cell face), crossing the cell face E in the physical domain. Eqn. 5.47 is multiplied by ΔS_E , then the result is equated to $F_{1_E} \Delta \eta$ according to Eqn. 5.46, and the numerical flux based on the Roe scheme is obtained in generalized coordinates. This is explained as follows.

To obtain total-mass, momentum or energy crossing the face E , Eqn. 5.47 is multiplied by ΔS_E :

$$R_{E_n} \Delta S_E = \frac{1}{2} [R_{E_n}^L \Delta S_E + R_{E_n}^R \Delta S_E] - \frac{1}{2} \sum_{\kappa=1}^4 |\hat{\lambda}_E^{(\kappa)}| \delta w_E^{(\kappa)} \hat{T}_E^{(\kappa)} \Delta S_E. \quad (5.48)$$

The L.H.S. of Eqn. 5.48 is replaced by $F_{1_E} \Delta \eta$ according to Eqn. 5.46. The other terms of Eqn. 5.48 (the terms in the R.H.S) are explicated in terms of the grid geometry and flow parameters. Therefore the numerical flux F_{1_E} is obtained. This procedure is explained as follows.

5.7 Right Hand Side of Eqn. 5.48

5.7.1 $R_{E_n}^L \Delta S_E$ or $R_{E_n}^R \Delta S_E$

Before obtaining $R_{E_n}^L \Delta S_E$ (or $R_{E_n}^R \Delta S_E$), it is appropriate to distinguish the difference between the terms $R_{E_n}^L \Delta S_E$ (or $R_{E_n}^R \Delta S_E$) with $R_{E_n} \Delta S_E$. $R_{E_n} \Delta S_E$ is the actual total-mass, momentum and energy crossing the face E predicted by the Roe scheme. In contrast, $R_{E_n}^L \Delta S_E$ (or $R_{E_n}^R \Delta S_E$) is a virtual (non-real) value for the total-mass, momentum and energy determined at flow conditions L or R . Eqn. 5.46 is a general equation and applies for all the flow conditions including inner and outer conditions L and R . Therefore,

$$R_{E_n}^L \Delta S_E = F_{1E}^L \Delta \eta \quad (5.49)$$

$$R_{E_n}^R \Delta S_E = F_{1E}^R \Delta \eta \quad (5.50)$$

5.7.2 L and R Flow Conditions

The flow conditions (L) and (R) at the cell face E can be determined in accordance with the degree of accuracy (first order, second order, etc.) and the type of scheme used (central, upwind, etc.). In this study only upwind schemes are considered.

(1) The first order upwind algorithm (upwinding) suggests that:

$$q_E^L = q_{j,k} \quad (5.51)$$

where q is a typical primitive variable, i.e. $q \in \{\rho, p, u, v\}$ or $q \in \{T, p, u, v\}$. For the first order extrapolation a zero-order polynomial (a straight flat line) is used to extrapolate the primitive variable q at node (j, k) to the cell face E . Fig. 5.13 shows the extrapolation of a typical primitive variable by first order upwinding.

(2) Second order upwinding recommends:

$$q_E^L = q_{j,k} + \frac{1}{2} \Delta_W q \quad (5.52)$$

where $\Delta_W q$ is the jump of a primitive variable at the west face of the control volume, i.e. $\Delta_W q = (q_{j,k} - q_{j-1,k})$. This gives:

$$q_E^L = \frac{1}{2} (3q_{j,k} - q_{j-1,k}). \quad (5.53)$$

For the second order extrapolation a first-order polynomial, i.e. a straight line, is used to extrapolate the primitive variable q from nodes $(j-1, k)$ and (j, k) to the cell face E , as shown in Fig. 5.14.

(3) A third order upwind-biased algorithm proposes:

$$q_E^L = q_{j,k} + \frac{1}{4}[(1 - \kappa)\Delta_W q + (1 + \kappa)\Delta_E q] \quad (5.54)$$

where $\kappa = \frac{1}{3}$ and $\Delta_E q$ is the jump of the primitive variable at E , i.e. $\Delta_E q = q_{j+1,k} - q_{j,k}$. This gives:

$$q_E^L = \frac{1}{6}(-q_{j-1,k} + 5q_{j,k} + 2q_{j+1,k}) \quad (5.55)$$

It is noted that for the third order extrapolation a second-order polynomial, i.e. a parabola, is used to determine the primitive variable q at the cell face E , as shown in Fig. 5.15. That is, a second order polynomial curve fit between the points $(j-1, k)$, (j, k) and $(j+1, k)$ is used to obtain q_E^L . This task is performed via Eqn. 5.54. The R side flow condition is determined in a similar manner as follows. For the first order approximation:

$$q_E^R = q_{j+1,k}, \quad (5.56)$$

for the second order approximation:

$$q_E^R = q_{j+1,k} - \frac{1}{2}\Delta_{EE}q \quad (5.57)$$

where $\Delta_{EE}q = q_{j+2,k} - q_{j+1,k}$, and for the third order upwind-biased approximation:

$$q_E^R = q_{j+1,k} - \frac{1}{4}[(1 - \kappa)\Delta_{EE}q + (1 + \kappa)\Delta_E q]. \quad (5.58)$$

In this chapter and the next chapter, a third order upwind-biased for the spatial discretization of convective and pressure terms will be used to determine the primitive variables at the L and R sides of the cell faces. It is noted for the higher order, i.e. higher than first order accurate cases, the solution is not necessarily monotone and non-physical oscillations are produced, which must be damped. To damp the numerical oscillations, the van Albada flux limiter (1982) is used.

5.7.3 Roe's Averaging

Once L and R conditions at face E are obtained, Roe's averaged condition is determined as follows: (For the formulation of the Roe scheme in the physical domain, the reader is referred to Appendix D)

$$\hat{\rho}_E \equiv W_E^L W_E^R \quad (5.59)$$

$$\hat{u}_E \equiv \frac{W_E^L u_E^L + W_E^R u_E^R}{W_E^L + W_E^R} \quad (5.60)$$

$$\hat{v}_E \equiv \frac{W_E^L v_E^L + W_E^R v_E^R}{W_E^L + W_E^R} \quad (5.61)$$

$$\hat{H}_E \equiv \frac{W_E^L H_E^L + W_E^R H_E^R}{W_E^L + W_E^R} \quad (5.62)$$

where

$$W_E^L = \sqrt{\rho_E^L}, \quad W_E^R = \sqrt{\rho_E^R}. \quad (5.63)$$

Therefore, other primitive variables, e.g. p_E , T_E , etc., corresponding to the L and R flow conditions could be obtained.

5.7.4 $\hat{\lambda}_E$, $\hat{T}_E$, and δw_E

Other terms of Eqn. 5.48, i.e. $\hat{\lambda}_E$, $\hat{T}_E$, and δw_E , are described as follows:

$$\begin{bmatrix} \hat{\lambda}_E^{(1)} \\ \hat{\lambda}_E^{(2)} \\ \hat{\lambda}_E^{(3)} \\ \hat{\lambda}_E^{(4)} \end{bmatrix} = \begin{bmatrix} \hat{u}_{\perp E} - \hat{c}_E \\ \hat{u}_{\perp E} \\ \hat{u}_{\perp E} \\ \hat{u}_{\perp E} + \hat{c}_E \end{bmatrix}, \quad \delta W_E \equiv \begin{bmatrix} \delta w_E^{(1)} \\ \delta w_E^{(2)} \\ \delta w_E^{(3)} \\ \delta w_E^{(4)} \end{bmatrix} = \begin{bmatrix} \frac{\delta p_E - \hat{\rho}_E \hat{c}_E \delta u_{\perp E}}{2 \hat{c}_E^2} \\ \hat{\rho}_E \delta u_{\parallel E} \\ - \frac{\delta p_E - \hat{c}_E^2 \delta \rho_E}{\hat{c}_E^2} \\ \frac{\delta p_E + \hat{\rho}_E \hat{c}_E \delta u_{\perp E}}{2 \hat{c}_E^2} \end{bmatrix} \quad (5.64)$$

and

$$\hat{T}_E^{(1)} = \begin{bmatrix} 1 \\ \hat{u}_E - \hat{c}_E \cos \theta_E \\ \hat{v}_E - \hat{c}_E \sin \theta_E \\ \hat{H}_E - \hat{u}_{\perp E} \hat{c}_E \end{bmatrix}, \quad \hat{T}_E^{(2)} = \begin{bmatrix} 0 \\ -\sin \theta_E \\ \cos \theta_E \\ \hat{u}_{\parallel E} \end{bmatrix},$$

$$\hat{T}_E^{(3)} = \begin{bmatrix} 1 \\ \hat{u}_E \\ \hat{v}_E \\ \frac{\hat{u}_E^2 + \hat{v}_E^2}{2} \end{bmatrix}, \quad \hat{T}_E^{(4)} = \begin{bmatrix} 1 \\ \hat{u}_E + \hat{c}_E \cos \theta_E \\ \hat{v}_E + \hat{c}_E \sin \theta_E \\ \hat{H}_E + \hat{u}_{\perp E} \hat{c}_E \end{bmatrix} \quad (5.65)$$

where $u_{\parallel E}$ is the velocity component parallel to face E obtained from $u_{\parallel E}^2 = \vec{V}_E \cdot \vec{V}_E - u_{\perp E}^2$, $\hat{c}_E$ is the speed of sound determined at Roe's averaged condition from:

$$\hat{c}_E = \sqrt{(\gamma - 1) \left(\hat{H}_E - \frac{1}{2} (\hat{u}_E^2 + \hat{v}_E^2) \right)}, \quad (5.66)$$

and $\delta \rho_E = \rho_{j+1,k} - \rho_{j,k}$, $\delta p_E = p_{j+1,k} - p_{j,k}$, $\delta u_{\parallel E} = u_{\parallel j+1,k} - u_{\parallel j,k}$ and $\delta v_{\perp E} = v_{\perp j+1,k} - v_{\perp j,k}$.

5.7.5 Numerical Flux for the Roe Scheme in Generalized Coordinates

Finally the numerical flux based on the Roe scheme in generalized coordinates is given in this section. Considering Eqns. 5.46, 5.49 and 5.50 also replacing ΔS_E from Eqn. 5.18, Eqn. 5.48 becomes:

$$F_{1E} \Delta \eta = \frac{1}{2} [F_{1E}^L \Delta \eta + F_{1E}^R \Delta \eta] - \frac{1}{2} \sum_{\kappa=1}^4 |\hat{\lambda}_E^{(\kappa)}| \delta w_E^{(\kappa)} \hat{T}_E^{(\kappa)} \left[\frac{\sqrt{\xi_x^2 + \xi_y^2}}{J} \right]_E \Delta \eta, \quad (5.67)$$

Once $\Delta \eta$ is canceled from both sides, the numerical flux F_{1E} crossing the face E of the computational cell, see Fig. 5.6 (Right), is obtained:

$$F_{1E} = \frac{1}{2} [F_{1E}^L + F_{1E}^R] - \frac{1}{2} \sum_{\kappa=1}^4 |\hat{\lambda}_E^{(\kappa)}| \delta w_E^{(\kappa)} \hat{T}_E^{(\kappa)} \left[\frac{\sqrt{\xi_x^2 + \xi_y^2}}{J} \right]_E. \quad (5.68)$$

Eqn. 5.68 represents the numerical flux based on the Roe scheme in generalized coordinates. Obtaining Roe's numerical flux in generalized coordinates has been the main message of this chapter. This task is completed by deriving Eqn. 5.68. Different forms for the numerical flux based on the Roe scheme are reported in the literature, a review of which is included here.

The solution of the Riemann problem in multi-dimensions has been carried out with some success, but this success has been limited by computational cost, complexity of the proposed models etc. (see Powell et. al. (1990) and Parpia and Michelak

(1993)). A comprehensive review in this regard is given by van Leer (1992). One recent method to solve the Riemann problem in multi-dimension is to rotate the local coordinate system (see Powell et. al. (1990)). Kontinos and McRae (1994) have also applied the locally rotated axis to some test cases with some success, however it is not clear that the improvement in accuracy justifies the additional complexity (see Tannehill et. al. (1997)). For example, as indicated by Powell et. al. (1990), the rotated Riemann solver for the higher-order schemes is denoted as not very impressive.

In either the case, to solve the Riemann problems in multi-dimension, the problem is solved normal to the cell faces with the relationship between the geometry of the cells. To the best knowledge of the author, the numerical flux function for the Roe scheme as explained and derived in this thesis (which is given by Eqn. 5.68) is the most complete, clear and most importantly simple form to represent the Roe's numerical flux in generalized coordinates. For comparison purposes, the reader is referred to the formulae given by the text Tannehill et. al. (1997) and the Manual of the CFL3D code edited by Biedron and Rumsey (1998). In the formulation by Tannehill et. al. (1997) the flux limiter function is included in the formulae for the numerical flux, which adds extra complexity to the formula. However, in the current study the primitive variables are limited before the computation of the numerical flux function.

Similarly the numerical flux G_{1_N} at the north face of the control volume B , as shown in Fig. 5.6, could be determined as follows:

$$G_{1_N} = \frac{1}{2} [G_{1_N}^L + G_{1_N}^R] - \frac{1}{2} \sum_{\kappa=1}^4 |\hat{\lambda}_N^{(\kappa)}| \delta w_N^{(\kappa)} \hat{T}_N^{(\kappa)} \left[\frac{\sqrt{\eta_x^2 + \eta_y^2}}{J} \right]_N, \quad (5.69)$$

where the superscript L and R correspond to inner and outer states at the cell face N , and

$$\begin{bmatrix} \hat{\lambda}_N^{(1)} \\ \hat{\lambda}_N^{(2)} \\ \hat{\lambda}_N^{(3)} \\ \hat{\lambda}_N^{(4)} \end{bmatrix} = \begin{bmatrix} \hat{u}_{\perp N} - \hat{c}_N \\ \hat{u}_{\perp N} \\ \hat{u}_{\perp N} \\ \hat{u}_{\perp N} + \hat{c}_N \end{bmatrix}, \quad \delta W_N \equiv \begin{bmatrix} \delta w_N^{(1)} \\ \delta w_N^{(2)} \\ \delta w_N^{(3)} \\ \delta w_N^{(4)} \end{bmatrix} = \begin{bmatrix} \frac{\delta p_N - \hat{\rho}_N \hat{c}_N \delta u_{\perp N}}{2 \hat{c}_N^2} \\ \hat{\rho}_N \delta u_{\parallel N} \\ - \frac{\delta p_N - \hat{c}_N^2 \delta \rho_N}{\hat{c}_N^2} \\ \frac{\delta p_N + \hat{\rho}_N \hat{c}_N \delta u_{\perp N}}{2 \hat{c}_N^2} \end{bmatrix} \quad (5.70)$$

and

$$\begin{aligned}
\hat{T}_N^{(1)} &= \begin{bmatrix} 1 \\ \hat{u}_N - \hat{c}_N \cos \beta_N \\ \hat{v}_N - \hat{c}_N \sin \beta_N \\ \hat{H}_N - \hat{u}_{\perp N} \hat{c}_N \end{bmatrix}, & \hat{T}_N^{(2)} &= \begin{bmatrix} 0 \\ -\sin \beta_N \\ \cos \beta_N \\ \hat{u}_{\parallel N} \end{bmatrix}, \\
\hat{T}_N^{(3)} &= \begin{bmatrix} 1 \\ \hat{u}_N \\ \hat{v}_N \\ \frac{\hat{u}_N^2 + \hat{v}_N^2}{2} \end{bmatrix}, & \hat{T}_N^{(4)} &= \begin{bmatrix} 1 \\ \hat{u}_N + \hat{c}_N \cos \beta_N \\ \hat{v}_N + \hat{c}_N \sin \beta_N \\ \hat{H}_N + \hat{u}_{\perp N} \hat{c}_N \end{bmatrix} \quad (5.71)
\end{aligned}$$

where all *hat* states denote Roe's averaged condition determined at the N face, $\cos \beta_N$ and $\sin \beta_N$ are given by Eqns. 5.13 and 5.14, $\delta \rho_N = \rho_{j,k+1} - \rho_{j,k}$, $\delta p_N = p_{j,k+1} - p_{j,k}$, $\delta u_{\parallel N} = u_{\parallel,j,k+1} - u_{\parallel,j,k}$, $\delta v_{\perp N} = v_{\perp,j,k+1} - v_{\perp,j,k}$ and $\hat{c}_N = \sqrt{(\gamma - 1) \left(\hat{H}_N - \frac{1}{2} (\hat{u}_N^2 + \hat{v}_N^2) \right)}$.

5.8 Discussion and Conclusion

The direct solution of the fluid equations with the Roe's scheme in the physical domain (finite-volume based solution in the physical domain) has been frequently reported in the literature, see for example Mazaheri and Abbasian (1998), Currie (1998) and Frink et. al. (1991). When Roe's scheme is applied over quadrilateral grids, there is no advantage of directly solving the fluid equations vs. that of solving the fluid equations in the transformed domain of computation, i.e. generalized coordinates. Moreover, the selection of quadrilateral grids for the Roe scheme is a more appropriate choice. Because, these kinds of grids are better able to be aligned with the flow, they produce less numerical diffusion. This is as opposed to triangular grids, which inevitably are almost always oblique to the whole flow field, therefore, producing unnecessary numerical diffusion which reduces the non-diffusive benefits of Roe's scheme.

There are only a few reports available in the literature on the formulation of the Roe scheme in generalized coordinates, and most of them are very brief (see Tannehill et. al. (1997) and CFL3D Manual edited by Biedron and Rumsey (1998)).

None of these reports have explained and shown the numerical flux for the Roe scheme in generalized coordinates as clearly and explicitly as shown here, given by Eqns. 5.68 and 5.69. In most of the formulations that could be found in the literature for the numerical flux for the Roe scheme in generalized coordinates, mixed terms some from the physical domain and some from the computational domain (or generalized coordinates) are included in the formulation for the numerical flux. However, Eqns. 5.68 and 5.69 contain only parameters relating exclusively to the generalized coordinates (i.e. metrics of transformation). For example, the skewness (or the cosine directions) of the control volume faces, which are used in obtaining of Eqns. 5.68 and 5.69 are explained merely based on the metrics of transformation. Another example is the area of the control volume faces, as given by Eqns. 5.18 and 5.19. The simplicity of the approach taken here and clarity of Eqns. 5.68 and 5.69 are the unique feature that have led us to obtain Eqns. 5.68 and 5.69.

The numerical flux for the Roe scheme as given by Eqns. 5.68 and 5.69, are applied to wide range of applications ranging from inviscid to viscous and turbulent flows as given in Chapter 6.

Figure 5.1: Schematic picture of inviscid shear flow (slipline).

Figure 5.2: Mach number distribution along the transverse direction at $x = -0.3, 0.0, 0.3, 0.6, 0.9$ after convergence is obtained. All the profiles overlap on a single profile.

Figure 5.3: Comparison of triangular grid with quadrilateral H for the grid alignment purposes.

Figure 5.4: Grid configuration in the physical domain (left) and computational domain (right).

Figure 5.5: Body fitted grid system with the unit vectors normal to the grid lines.

Figure 5.9: Components of the velocity vector $\vec{V}_E$.

Figure 5.10: Schematic of: (1) $\Delta \vec{S}_E$, (2) $\vec{R}_E$ and its component along $\Delta \vec{S}_E$, (3) unit vector $\hat{n}_E$ along $\Delta \vec{S}_E$.

Figure 5.11: Schematic of $\vec{V}_E$ and its components in directions either: (1) x - y or (2) parallel and normal.

Figure 5.12: Inner (L) and outer (R) values associated with a cell face. Grid lines are shown by solid lines and control volume boundaries with dashed-lines.

Figure 5.13: The cell face value L is determined by the first order upwinding ($q_E^L = q_j$).

Figure 5.14: The cell face value L is determined by the second order upwinding ($q_E^L = q_j + \frac{1}{2}\Delta_W q$; $\Delta_W q = (q_j - q_{j-1})$).

Figure 5.15: The cell face value L as determined by the third order upwind-biased extrapolation.

Chapter 6

Roe Scheme in Generalized Coordinates; Application to Inviscid and Viscous Flows

6.1 Introduction

The formulation for the numerical flux resulting from use of the Roe scheme in generalized coordinates as outlined in Chapter 5 of this thesis, is now assessed by applying it to several inviscid and viscous test cases.

For the spatial discretization of convective and pressure terms, the primitive variables (pressure, temperature and velocity components) are extrapolated to the cell faces by the MUSCL idea using the third order upwind biased scheme. The van Albada flux limiter is used to prevent spurious numerical oscillations. The viscous terms are centrally differenced.

In Chapter 5, fluid equations in the physical domain and in the computational domain are put side by side, term by term and a formula is obtained to give the numerical flux for the Roe scheme in generalized coordinates. This numerical flux is written in terms of grid-geometry (metrics of transformation from the physical domain to the computational domain) and the flow parameters (see Chapter 5 or Kermani and Plett (2001^b) for more detail). That method is now assessed in this

chapter by application to some inviscid and viscous test cases as also outlined in Kermani and Plett (2001^c).

6.2 Governing Equations

The fluid equations for the viscous, unsteady and compressible flow in full conservative form in generalized coordinates with no body force could be approximated by thin layer Navier-Stokes equations as follows, see Hoffmann and Chiang (1993) for example:

$$\frac{\partial Q_1}{\partial t} + \frac{\partial F_1}{\partial \xi} + \frac{\partial G_1}{\partial \eta} = \frac{\partial G_{1v_T}}{\partial \eta} \quad (6.1)$$

where Q_1 is the conservative vector, F_1 and G_1 are the inviscid flux vectors, and G_{1v_T} is the viscous flux vector obtained with the thin-layer approximation, all determined in generalized coordinates. The thin-layer approximation is suitable for high speed flows, in which all the viscous derivatives along the main stream of the flow, such as along ξ , are neglected. Eqn. 6.1 is discretized over the control volume (j, k) as shown in Fig. 6.1 as follows:

$$\frac{\partial \tilde{Q}_1}{\partial t} + \frac{F_{1E} - F_{1W}}{\Delta \xi} + \frac{G_{1N} - G_{1S}}{\Delta \eta} = \frac{G_{1v_{TN}} - G_{1v_{TS}}}{\Delta \eta} \quad (6.2)$$

where F_{1E} is the inviscid numerical flux obtained in generalized coordinates at the east face of the cell, E , as described in Chapter 5, F_{1W} , G_{1N} and G_{1S} are the inviscid fluxes at the west, north and south cell faces respectively and $G_{1v_{TN}}$ and $G_{1v_{TS}}$ are the viscous fluxes obtained at the north and south faces of the control volume. According to the thin-layer approximation, the difference between the east and west terms of the viscous fluxes are small relative to the north and south viscous fluxes and approximately cancel each other.

6.3 Presentation of Numerical Flux by the Roe Scheme in Generalized Coordinates

The inviscid numerical flux F_{1E} based on the Roe scheme is written in generalized coordinates, according to Chapter 5 as:

$$F_{1E} = \frac{1}{2} [F_{1E}^L + F_{1E}^R] - \frac{1}{2} \sum_{\kappa=1}^4 |\hat{\lambda}_E^{(\kappa)}| \delta w_E^{(\kappa)} \hat{T}_E^{(\kappa)} \left[\frac{\sqrt{\xi_x^2 + \xi_y^2}}{J} \right]_E \quad (6.3)$$

where F_{1E}^L and F_{1E}^R are the inner and outer values of F_1 determined at face E , $\hat{\lambda}_E$'s are the eigenvalues of the Jacobian matrix determined at Roe's averaged condition, δw_E 's are the wave amplitude and $\hat{T}_E$'s are the eigenvectors corresponding to the eigenvalues ($\hat{\lambda}_E$'s) determined at Roe's averaged conditions. For a complete description of these parameters the reader is referred to Chapter 5 or Kermani and Plett (2001^b). F_{1W} is equal to F_{1E} at the previous node in the ξ direction. G_{1N} is determined in the same manner as for Eqn. 6.3, as described in Chapter 5. The viscous fluxes are obtained by central differencing.

6.4 Time Discretization

For the time discretization, the following two-step explicit scheme, from the Lax-Wendroff family of predictor-corrector, is used, as outlined in section 2.3.3 for one-dimensional inviscid flow and repeated here for the thin-layer Navier-Stokes equations in brief. The predictor step provides the flow condition in an intermediate step $n + 1/2$.

$$\frac{Q_1^{n+1/2} - Q_1^n}{\Delta t/2} + \left(\frac{\partial F_1}{\partial \xi} \right)^n + \left(\frac{\partial G_1}{\partial \eta} \right)^n = \left(\frac{\partial G_{1v_T}}{\partial \eta} \right)^n \quad (6.4)$$

Eqn. 6.4 gives $Q_1^{n+1/2}$, from which all the primitive variables at the time step $n + 1/2$ could be determined. The predictor step is followed by the corrector step, which completes the time integration. In the corrector step, a central differencing in time around $n + 1/2$ is implemented as follows:

$$\frac{Q_1^{n+1} - Q_1^n}{\Delta t} + \left(\frac{\partial F_1}{\partial \xi} \right)^{n+1/2} + \left(\frac{\partial G_1}{\partial \eta} \right)^{n+1/2} = \left(\frac{\partial G_{1v_T}}{\partial \eta} \right)^{n+1/2} \quad (6.5)$$

for which F_1 , G_1 and G_{1v_T} are calculated by using the primitive variables obtained by solving Eqn. 6.4 at the half time step.

6.5 Space Discretization

In this computation a third order upwind-biased algorithm with the MUSCL extrapolation strategy of van Leer (1979), is applied to the primitive variables pressure (p), velocity components (u, v) and temperature (T), in order to obtain the inner (L) and outer (R) flow conditions. For example at the east cell face of the control volume, E , the L and R flow conditions are determined as follows:

$$\begin{aligned} q_E^L &= q_{j,k} + \frac{1}{4}[(1 - \kappa)\Delta_W q + (1 + \kappa)\Delta_E q] \\ q_E^R &= q_{j+1,k} - \frac{1}{4}[(1 - \kappa)\Delta_{EE} q + (1 + \kappa)\Delta_E q], \end{aligned} \quad (6.6)$$

where q represents a primitive variable, i.e. either (p, u, v, T) , and $\kappa = 1/3$ for the current study as the third order upwind biased scheme and: $\Delta_W q = q_{j,k} - q_{j-1,k}$, $\Delta_E q = q_{j+1,k} - q_{j,k}$ and $\Delta_{EE} q = q_{j+2,k} - q_{j+1,k}$.

In the current computations, the van Albada et. al. flux limiter (1982), is applied. This limiter has been reported and implemented in two different forms in the literature. The first approach as implemented for example by Thomas and Walters (1987), recommends:

$$\begin{aligned} q_E^L &= q_{j,k} + \frac{\phi}{4}[(1 - \kappa\phi)\Delta_W q + (1 + \kappa\phi)\Delta_E q] \\ q_E^R &= q_{j+1,k} - \frac{\phi}{4}[(1 - \kappa\phi)\Delta_{EE} q + (1 + \kappa\phi)\Delta_E q], \end{aligned} \quad (6.7)$$

where ϕ is the limiter function ($0 \leq \phi \leq 1$), which is a function of forward- and backward-differences, as defined by:

$$\phi_{j,k} \equiv \frac{2(\Delta_W q)(\Delta_E q) + \epsilon}{(\Delta_W q)^2 + (\Delta_E q)^2 + \epsilon} \quad (6.8)$$

and ϵ is a small number which prevents indeterminacy in regions of uniform flow, i.e. in regions $(\Delta_W q) = (\Delta_E q) = 0$. The flux limiter extrapolation formulation given by Eqn. 6.7 cannot totally prevent the spurious numerical oscillations. Alternatively, it is found that the following form of this flux limiter is better able to prevent the

spurious numerical oscillations and give better convergence. This is based on two separate personal communications with Dr. Amaladas of the Indian Institute of Technology (2000) and Dr. Thomas of NASA Langley (2000), both recommending the following formulae for the extrapolation of the primitive variables:

$$\begin{aligned} q_E^L &= q_{j,k} + \frac{\phi}{4}[(1 - \kappa)\Delta_W q + (1 + \kappa)\Delta_E q] \\ q_E^R &= q_{j+1,k} - \frac{\phi}{4}[(1 - \kappa)\Delta_{EE} q + (1 + \kappa)\Delta_E q]. \end{aligned} \quad (6.9)$$

Eqn. 6.9 has been used throughout this thesis for the extrapolation of primitive variables.

To avoid expansion shocks from appearing in those regions of sonic expansions the following entropy correction formula, as outlined in Chapter 4 and by Kermani and Plett (2001^a), is used throughout this thesis.

$$\begin{cases} \hat{\lambda}_{new} \leftarrow \frac{\hat{\lambda}^2 + \epsilon^2}{2\epsilon} & |\lambda| < \epsilon \\ \epsilon = 4.0 \max \left[0, (\hat{\lambda} - \lambda^L), (\lambda^R - \hat{\lambda}) \right], \end{cases} \quad (6.10)$$

where $\hat{\lambda}$ is the eigenvalue of the Jacobian flux matrix determined at Roe's averaged condition (see appendix D), and λ^L and λ^R are the eigenvalues determined at inner or outer flow conditions, respectively.

6.6 Inviscid Flow Test Cases

The numerical flux based on the Roe scheme in generalized coordinates, as outlined in Chapter 5, has been applied to the following inviscid test cases: (1) Supercritical flow over a bump, and (2) inviscid transonic flow in a converging-diverging nozzle, also called a De Laval nozzle. A complete explanation of these test cases are given in Chapter 4 and are not repeated here. In both of these test cases, subsonic flow accelerates to supersonic flow and a terminating normal shock returns the flow to subsonic flow. Both of these test cases contain regions of sonic expansion, i.e. local *Mach* number 1. The expansion shocks are avoided by the entropy correction formula as given by Eqn. 6.10. The accuracy assessment for these cases show excellent

agreement with analytical results and computations by others, see Chapter 4 for comparison purposes.

6.7 Blasius Flow

The first viscous flow validation case is the viscous incompressible laminar flow over a flat plate at zero angle of incidence. The results of this test are compared with the analytic results of Blasius. The Mach number of the free stream is 0.5 and the Reynolds number based on the length measured from the leading edge of the plate is 10,000. The geometry of the plate is shown in Fig. 6.2. The flat plate has a length L and the computational domain is extended a distance $L/2$ upstream of the leading edge. This distance allows the flow to develop from the uniform inflow condition as it approaches the plate.

The number of grids for this test case are 31 along the plate (including grids ahead of the plate) and 21 in the transverse direction (with clustering factor 1.7), as shown in Fig. 6.3. The grid was generated by an algebraic grid generator code. An initial condition, which is the same as the free stream condition is applied for this problem. The boundary conditions are as follows. Inflow conditions of uniform total pressure and total temperature with zero transverse velocity component were applied at the inlet to the computational domain. Outflow conditions corresponding to the free stream pressure at the top and downstream boundary of the computational domain were specified. No slip adiabatic wall conditions were specified on the plate with symmetry conditions applied across the extended plane ahead of the plate.

The classical Blasius similarity solution provides data for comparison. The text by White (1991) discusses this solution. The computed velocity component along the plate, u , is compared with that of the Blasius solution as shown in Fig. 6.4. In the current computation the boundary layer has been accurately captured within 8 grid points by the third order upwind biased scheme as applied to Roe's algorithm in generalized coordinates. Using the same grid, with the first order scheme, the boundary layer profile has also been captured fairly well everywhere except at the outer edge of the layer. Using the van Leer flux vector splitting algorithm with the

third order upwind-biased scheme in the same flow condition, i.e. $Mach=0.5$ and Reynolds number 10,000, at least 20 nodes were required within the boundary layer in order to reasonably capture the boundary layer profile, see Thomas and Walters (1987). The first order upwind scheme of van Leer was totally incapable of capturing the boundary layer profile with this number of nodes, in which the boundary layer thickness was predicted to be four to five times larger than that of Blasius solutions (see Thomas and Walters (1987)).

This present success is due to the non-diffusive property of the Roe scheme, which makes it suitable of the viscous flow computations. A comparison for the level of diffusivity of various upwind and central numerical schemes such as those of van Leer's flux vector splitting (1982), Roe's flux difference splitting (1981), McCormack's explicit-implicit scheme (1982), and Jameson's central scheme (1981), is performed by van Leer et. al. (1987). In his paper it is concluded that Roe's numerical scheme is the most suitable algorithm for the viscous flow computation, as it is less-diffusive, of those which he had studied.

In the computation of the laminar flow over the flat plate discussed in this chapter, the wall skin friction factor for the laminar flow over the flat plate is also compared to that of Blasius exact solution in Fig. 6.5. As shown in these figures the agreement is very good.

6.8 Plane Poiseuille Flow

The next validation test is the laminar incompressible flow between two parallel plates as shown in Fig. 6.6. The fully developed flow between the plates is compared with the analytic results of plane Poiseuille flow.

In this example, the plates have a length 0.024 meter (2.40 *cm*) and are separated by 1.6×10^{-4} meter. The leading edges of the plates are located at $x = 0.0$. The computational domain is extended to some distance upstream of the leading edges of the plates where uniform inflow is specified.

In this example, flow with average velocity $\approx 26 \frac{m}{s}$ enters the domain of computation. This flow gradually develops as it approaches the plates. Over each plate

a boundary layer develops and thickens along the plate until the boundary layers from two plates meet each other at some distance from the leading edge of the plate, L_e . L_e is the flow development region (also called entrance length). For $x \geq L_e$, the velocity profile remains unchanged with x and flow is called *fully developed*. In the fully developed region a linear pressure drop in the flow direction is expected.

The flow conditions at the inlet plane are set to: $p_{0,in}=107,827 \text{ Pa}$, $T_{0,in}=292.2 \text{ }^\circ\text{K}$, and $\Phi=0$, where $p_{0,in}$ and $T_{0,in}$ are the total pressure and temperature and Φ is the flow angle. The Reynolds number in this test case based on the inflow condition and the hydraulic diameter, D_h , is: $Re_{D_h} = \rho_{in} u_{in} D_h / \mu_{in} \approx 575$, where $D_h = 2h$ for a channel consisting of two parallel plates extending to infinity in the z direction (see Fig. 6.6). The Reynolds number of 575 in this problem is well below the critical Reynolds number, 2300, so the flow could be safely assumed to be laminar.

Due to the flow symmetry above and below the centerline only half of the geometry is computed here. In this study 201×45 uniform grid are taken along the plate and in the transverse direction, respectively. A uniform initial condition of $p = 101300 \text{ Pa}$, $T = 287 \text{ }^\circ\text{K}$ with $Mach = 0.3$ is applied for this problem.

Conditions corresponding to the pressure $p = 101300 \text{ Pa}$ at the outlet of the computational domain were specified. No slip adiabatic wall conditions were specified on the plate with the symmetry conditions ahead of the plate. The symmetry condition also has been applied at the center plane between the plates.

6.8.1 Results and Comparisons

The analytical solution of the plane Poiseuille flow are taken for comparison with the results obtained from the current study in the fully developed region. The text by White (1991) discusses the analytical solution of plane Poiseuille flow in which the velocity profile in the fully developed region is determined as follows. The x-momentum Navier-Stokes equations in the fully developed region are simplified to: $0 = -\frac{\partial p}{\partial x} + \mu \frac{\partial^2 u}{\partial y^2}$. For p as a function of only x , and u a function of only y , it is concluded that: $\frac{\partial p}{\partial x} = \mu \frac{\partial^2 u}{\partial y^2} = \text{constant}$. Therefore, $\frac{\partial}{\partial x} = \frac{d}{dx}$ and $\frac{\partial}{\partial y} = \frac{d}{dy}$ in the fully developed region. Hence, $0 = -\frac{dp}{dx} + \mu \frac{d^2 u}{dy^2}$. The boundary conditions are: $u = 0$

at the bottom wall ($y = 0$), and $\frac{du}{dy} = 0$ at the centerline ($y = \frac{h}{2}$), see Fig. 6.6. Integrating the above equation twice and applying the boundary conditions yield the velocity profile in the fully developed region as:

$$u = \frac{1}{2\mu} \left[-\frac{dp}{dx}\right] y (h - y), \quad (6.11)$$

where $[-\frac{dp}{dx}]$ is the pressure gradient along the plate which is constant in the fully developed region. Eqn. 6.11 gives the analytical value for the velocity profile in the fully developed region. To compare the analytical velocity profile as given by Eqn. 6.11, with that of the current computation, the values for $\frac{dp}{dx}$, μ and h must be given to Eqn. 6.11. In the current computation the following values are taken:

$$\begin{aligned} h &= 1.6 \times 10^{-4} \text{ m} \\ \mu &= 1.813 \times 10^{-5} \frac{N \cdot s}{m^2}. \end{aligned} \quad (6.12)$$

The input value of $\frac{dp}{dx}$ to Eqn. 6.11 is taken from the pressure distribution at the center line of the two plates (obtained from the current computation), as shown in Fig. 6.7. As shown in Fig. 6.7, p varies linearly in the x -direction in the fully developed region providing a constant value for the $\frac{dp}{dx}$ in this region. This constant is:

$$\frac{dp}{dx} \approx -2.417 \times 10^5 \frac{Pa}{m}. \quad (6.13)$$

Substituting the values from Eqns. 6.12 and 6.13 in to Eqn. 6.11, the analytical velocity profile becomes:

$$u = 6.666 \times 10^9 y (1.6 \times 10^{-4} - y) \left[\frac{m}{s}\right]. \quad (6.14)$$

Comparison of the velocity profile obtained analytically to that of the current computation at the exit plane of the parallel plates is shown in Fig. 6.8, where the agreement may be seen to be very good.

6.9 Shock-Boundary Layer Interaction

The next test case presents a more severe test in which a shock wave interacts with a laminar boundary layer over the flat plate. This is a phenomenon of great

complication because the behavior of the boundary layer mostly depends on the Reynolds number, whereas the Mach number predominantly determines the conditions in the shock wave. In the current test case a shock wave interaction with a laminar boundary layer that develops on a flat plate is studied.

As shown in Fig. 6.9, an oblique shock enters the domain of interest and impinges on a laminar boundary layer on a flat plate. This shock is introduced as an incident shock in Fig. 6.9. If the incident shock has sufficient strength it will cause the boundary layer to separate at point *S*-upstream of the impingement point. The boundary layer downstream of the impingement point reattaches to the plate at *R*. This produces a separation bubble. This bubble looks like an imaginary inviscid bump to the main flow. Therefore, a sequence of processes are induced by this imaginary bump as follows; (1) compression waves caused by leading edge of the separation bubble (or the leading edge of the imaginary bump), (2) expansion fans caused by the turning of flow over around the peak points of the bubble (or from around the maximum thickness of imaginary bump) and (3)- re-compression waves to make the flow streams parallel to the wall after the stream passes the imaginary bump's maximum point. Both qualitative and quantitative study of the flow around this separation bubble are the foci of this section.

As shown in Fig. 6.9 the compression and re-compression waves approach each other, converging to each other and make a stronger wave. On the other hand the expansion fans diverge as depicted in Fig. 6.9. This portraiture agrees with the physics of traveling waves, as described here. Consider a simplified case of uni-dimensional flow containing a series of compression- or expansion-waves. For a sequence of compression waves, the front waves are always followed by the waves at higher temperature, which contain higher wave speeds. So compression waves overtake each other (converge on each other) making a stronger wave which could grow to be a shock wave. On the other hand, in a sequence of expansion waves the front waves are followed by waves at lower temperature containing lower wave speed. So expansion waves cannot catch up to those preceeding them so they diverge and form expansion fans.

Away from the separation bubble and around the leading edge of the plate,

a weak shock is generated from the boundary layer development. This shock is generated by the flow obstruction caused by the initial growth of the boundary layer.

The model problem corresponds to the experiments of Hakkinen et. al. (1959). This experiment was performed in an 8×8 -inch supersonic wind tunnel in the Gas Turbine Laboratory of the Massachusetts Institute of Technology. The tunnel was able to deliver a flow with a fixed $Mach = 2$. The Reynolds number range, based on the distance from the leading edge of the plate to the shock impingement point, was 1 to 6.0×10^5 .

Numerically simulating this determining test has been a challenge for the accuracy assessment of numerical schemes. Several people have assessed their numerical schemes and flow solvers against this case. To name a few: Beam and Warming (1978), MacCormack (1975), Thomas and Walters (1987), Liou and Steffen (1993), and Amaladas (1995). All of these researchers have studied a case corresponding to Reynolds number equal to 2.96×10^5 with the shock angle $\beta = 32.6^\circ$ and inflow $Mach = 2.00$. The same values for Mach number and Reynolds number are taken for the current study.

6.9.1 Computational Domain and Flow Description

The flat plate has a length of 9 *cm*. The leading edge of the plate is located at $x = 0.0$. The computational domain is extended to some distance upstream of the leading edge of the plate, say 6 *mm*. This distance allows the leading edge shock wave to form properly. The geometric configuration of the flow past the plate is shown in Fig. 6.10. As shown in this figure, L is the point that the incident shock impinges on the plate if the flow is assumed inviscid.

Two grid resolutions are used here. (1) A very fine grid, 201×201 , in order to completely capture the physical detail of the flow, and (2) some coarser grids for the grid independency tests, e.g. 85×99 and 41×49 .

Free stream conditions for this test case are taken as follows: $M_\infty = 2.00$, $p_\infty = 13$ *kPa* and $T = 288^\circ K$. The Reynolds number per unit length is: $5.98 \times 10^6 \text{ m}^{-1}$, or

$Re_L = 5.98 \times 10^6 L$. To compare the result of this study with the experiments of Hakkinen (1959) in which $Re_L = 2.96 \times 10^5$, we require $L=4.95$ cm, where L is the shock impingement point if the flow is inviscid.

6.9.2 Initial and Boundary Conditions

A uniform initial condition of $p=13$ kPa, $T = 288^\circ K$, with $M=2.00$ and flow angle $\phi = 0.0$ w.r.t. the x-axis are specified as the initial conditions for this problem.

The boundary conditions for this problem are as follows. At the supersonic inflow, all primitive variables were specified. The inflow plane is split into two parts. (1) Below the incident shock location, where free stream conditions: $p=13$ kPa, $T = 288^\circ K$, with $M=2.00$ and flow angle $\phi = 0.0$ are specified and (2) above the incident shock entrance location, where primitive variables corresponding to the post shock conditions are imposed. These post shock conditions are determined from Rankine-Hugoniot relations by selecting the shock angle $\beta = 32.6^\circ$ and the upstream Mach number equal to 2.00. That gives: $p_2/p_1=1.188$, $T_2/T_1=1.051$, $M_2=1.889$ and $\phi=3.108$. Therefore, the post shock conditions (conditions above the incident shock location at the inlet plane) are determined as follows: $p=15.444$ kPa, $T=302.688^\circ K$, $u=657.802 \frac{m}{s}$ and $v= -35.717 \frac{m}{s}$.

The exit plane is positioned far enough from the separation region so that all the gradients in the flow direction are set to zero. Although this condition is not exact, it can be justified as follows. The boundary layer equations close to the bottom wall are parabolic in type, which allows the exit plane condition to be safely determined from its history at the upstream neighborhood of the exit plane. The remainder of the flow in the exit plane is supersonic and its governing equations are hyperbolic. Therefore, setting the gradients of primitive variables along the plate at the exit plane equal to zero will not introduce significant error in the region of shock boundary layer interaction.

A no slip adiabatic wall condition was imposed on the solid wall at the bottom of the computational domain. Also, the symmetry condition is enforced ahead of the plate at the bottom of the computational domain. The top of the computational

domain is assumed to be far enough from region of interest so the reflected shocks and the leading edge shock totally remain inside the computational domain. This allows the same condition at the inlet plane as referred to post shock conditions, i.e. above the incident shock, to be enforced at the top boundary of the computational grid.

6.9.3 Results and Comparisons

A qualitative study of the shock boundary layer interaction is performed first. To completely capture the physical detail of the flow, a very dense grid, i.e. 201×201 , is taken. This provides enough nodes inside the separation bubble, ≈ 30 , in order to capture the profile of recirculating flow.

For the computation of this problem in the current study two types of the governing equations are used, namely, thin layer Navier-Stokes and full Navier-Stokes. For the grid types examined here and elsewhere (see Thomas and Walters (1987)) with a high aspect ratio of the grids in the vicinity of the wall (i.e. very coarse grid along the plate and fairly fine in transverse direction), no distinguishable difference between the results was observed. The results presented here are those using the thin layer Navier-Stokes equations.

Fig. 6.12 shows the density contours obtained from the current study. As shown in this figure, the incident shock is strong enough to cause the boundary layer to separate. The separated boundary layer reattaches somewhere downstream of the impingement point. To study the flow condition in and around the separation bubble, the region is split into two regions. (1) Outside the separation bubble, i.e. away from the circulating region and in the inviscid core, and (2) inside the separation bubble, as follows:

(1) Outside the Recirculating Region

Fig. 6.13 shows the velocity vector and streamline patterns in and around the separation bubble. The separation bubble, earlier called an imaginary inviscid bump, causes a sequence of compression waves, expansion fans and re-compression waves

to be generated, as depicted in Fig. 6.9. The influence and presence of the imaginary bump in the region away from the separation bubble (above the separation bubble) is studied here. The compression and expansion effects of these waves can be better seen if the pressure distribution is illustrated along a constant y line above the separation bubble. As shown in Fig. 6.13, the location of the center of the separation bubble is well below $y \approx 1 \text{ mm}$. Hence, $y=1 \text{ cm}$ is well above and outside the separation bubble. Fig. 6.11 shows the pressure distribution along $y = 1 \text{ cm}$. In this figure, the pressure jump due to the leading edge shock, incident shock, compression wave, expansion fans and re-compression waves are shown. The pressure rise in the compression wave, pressure drop in the expansion fan followed by the pressure rise in the re-compression waves are clearly shown in Fig. 6.11.

Referring to Fig. 6.12, the approach (or convergence) of compression waves and divergence of expansion fans as schematically sketched in Fig. 6.9 has also been correctly predicted in the current computation. This experience agrees well with the physical interpretation of the uni-directional flow for the compression waves (convergence of compression waves) and expansion fans (divergence of expansion waves) as explained earlier.

The weak shock generated by the initial growth of the boundary layer at the leading edge of the plate has also been captured in the current computation, as shown in Figs. 6.12 and 6.11.

(2) Inside the Recirculating Region

Near the point where the shock wave approaches the wall, i.e. in and around the recirculating zone, the rate of change of $\partial u/\partial x$ and $\partial v/\partial x$ become of the same order of magnitude and the pressure gradient in the transverse direction, $\partial p/\partial y$, can no longer be ignored. That is, the boundary layer approximation is not an appropriate assumption in this region any more. The physics of the flow inside the separation bubble is studied here. Fig. 6.14 shows the iso-bar lines near the place that the incident shock reaches the wall. The iso-bar lines are bent backward in this region. This phenomena is explained here by a close look at the pressure distribution in the vicinity of the wall.

Due to the no slip conditions at the solid boundary, the particles near the wall can only move with subsonic velocities, as opposed to the flow away from the wall, which can move supersonically. Therefore, the incident shock wave, which originated in the external stream, cannot reach right down to the wall. Hence, the iso-bar lines which originate as shock waves in the supersonic region, i.e. away from the wall, diffuse to compression waves near the wall in the subsonic region. This phenomena is shown in Fig. 6.14 and is explained as follows.

Upstream of the recirculating zone, the streamlines inside the boundary layer are parallel to that of the external flow just outside the boundary layer. Therefore, pressure inside the boundary layer is the same as that at the edge of the boundary layer. That is $\partial p / \partial y$ vanishes in this region. In other words, the boundary layer theory applies there. The same idea is true downstream of the recirculating region, where streamlines become parallel again to the contour of the body, after the flow re-attaches, and the boundary layer concept is applicable again. That is pressure inside the boundary layer matches the value just outside the boundary layer, i.e. $\partial p / \partial y \approx 0$ likewise upstream of the recirculating zone. The fact that boundary layer pressure is the same as that just outside the boundary layer both upstream and downstream of the separation bubble, requires that the pressure rise inside the boundary layer match that of the external flow.

Outside the boundary layer, in which supersonic flow exists, the presence of shock waves are allowed, and large gradients of pressure (or any other primitive variable) are permitted. On the other hand inside the subsonic region of the boundary layer, near the wall, shocks are not allowed. This makes the pressure rise near the wall to be more gradual than that of the external stream. This flattening of the pressure gradient in the subsonic region of the boundary layer is illustrated in Fig. 6.14, where the isobar lines exist as shock waves away from the wall but are diffused and made compression waves near the wall and, therefore, they are bent backward near the place that the shock approaches the wall. This phenomena is quite different from the inviscid flow in which shock waves can totally reach the solid wall, as shown in Fig. 6.15. Therefore, no diffusion of pressure gradient is observed near the wall for inviscid flow. Comparison of wall pressure distribution on the wall for viscous and

inviscid flows are shown in Fig. 6.16. Expectedly, the ultimate pressure rise in the viscous flow matches that of inviscid flow, as shown in Fig. 6.16, although pressure is significantly diffused for the viscous flow as opposed to the inviscid case. Also shown in Fig. 6.16, the pressure profile becomes almost level, flat, around the location that the shock wave approaches the wall. This is the plateau profile of pressure inside the recirculating region. More detail on the pressure distribution inside the separation bubble in the shock boundary layer interaction, is given by Hakkinen (1959)

Comparisons with Experimental Values

The quantitative study of the shock boundary layer interaction is given here. Fig. 6.17 shows the comparison of pressure distribution over the plate obtained by the current computation with that of experimental values. The agreements are excellent. Fig. 6.18 shows the comparison of skin friction over the plate obtained by the current computation with that of experimental values. The agreements are fairly good.

The test cases are performed in three different grid densities, 201×201 , 85×99 and 41×49 , in order to obtain a grid independent solution. The results shown in Figs. 6.17 and 6.18, show that results are fairly grid independent even with the most coarse grid, 41×49 . This is an interesting feature of the Roe scheme as a non-diffusive scheme, which allows that the solution become grid independent on a fairly coarse grid. This feature of the Roe scheme makes it suitable for the viscous flow computations. The same problem has been computed by the van Leer scheme as reported in Thomas and Walters (1987), in which 113 nodes were required in the transverse direction to achieve a grid independent solution.

6.10 Turbulent Flow Between Parallel Plates

The next turbulent computation is steady, turbulent channel flow of an incompressible fluid between parallel plates.

Two types of solutions for this flow are obtained and compared with each other:

- (i) an approximate analytical solution for the fully developed flow in a channel, and
- (ii) a computational result in a long enough channel, which allows the flow to be

fully developed. In the computational solution the entrance region has also been computed but here only comparisons are made for the region in which the flow is fully developed.

6.10.1 Geometry

The two parallel plates have the length $L=6.00$ meter and are apart from each other by $h=0.1$ meter. The leading edges of the plates are located at $x = 0.0$. The schematic geometry and computational box for this test case are shown in Figs. 6.6 and 6.19, respectively.

6.10.2 Flow Description

This is a subsonic test case with the stagnation pressure, $p_{0,in}$, the stagnation temperature, $T_{0,in}$, and with the flow angle at the inlet plane, Φ , specified. The exit pressure, p_e , is also specified here. The numerical values for $p_{0,in}$, $T_{0,in}$, Φ , and p_e are as follow. The exit pressure is set to ambient pressure, i.e. $p_e=101.3 \text{ kPa}$. $p_{0,in}$ corresponds to p_e and $Mach=0.3$. $T_{0,in}$ is obtained corresponding to an arbitrarily given reference temperature, say $320 \text{ }^\circ K$, and $Mach=0.3$. These conditions are summarized in the following table:

$p_{0,in} \text{ (kPa)}$	$T_{0,in} \text{ (}^\circ K\text{)}$	Φ
107.827	325.76	0.0

The Mach number of flow is ≈ 0.3 , which can be assumed incompressible. Over each plate a boundary layer develops and thickens along the plate until they meet each other at a distance L_e from the leading edges, where L_e is the flow development length. Various formulations were given for obtaining the fully developed length in turbulent duct flow, e.g. see Kays and Crawford (1993):

$$\frac{L_e}{D_h} = 0.623 R_{eD_h}^{0.25} \quad (6.15)$$

where D_h is the hydraulic diameter and R_{eD_h} is the Reynolds number based on D_h . For two parallel plates, $D_h =$ two times the gap between the plates, i.e. $D_h = 0.2$

meter for this case with the given flow condition

$$Re_{D_h} \approx 1.04 \times 10^6 \quad (6.16)$$

This is well above 2300 so the flow is fully turbulent. This gives $L_e \approx 3.98$ meter. The length of the computational box, $L=6.00$ meter, is $\approx 1.5 \times L_e$.

6.10.3 Computational Grid

Two grid densities are studied here: (i) 151 grid along the channel and 51 in the transverse direction with the clustering factor 1.001 near the bottom and top wall. This provides the y^+ of the first node above the wall to be 3.64 which is less than 5, where the sub-layer is usually assumed to end. In total, two nodes are within the sub-layer in this grid configuration including the node at the wall. (ii) 151 grids along the channel and 81 in the transverse direction with the same clustering factor 1.001 near the bottom and top wall. This provides the y^+ of the first node above the wall to be 2.12. This grid configuration provides three nodes within the sub-layer including the wall node.

Both of these grid resolutions provide enough nodes inside the sub-layer region, in which the velocity profile is linear, to capture a correct value for the wall shear stress.

6.10.4 Initial Conditions

A uniform initial condition of $p=101.3 \text{ kPa}$, $T=320^\circ K$ with $Mach = 0.3$ and the flow angle with x-axis $=0$, are applied for this problem.

6.10.5 Boundary Conditions

Inflow conditions of uniform total pressure and total temperature with zero vertical velocity were applied upstream of the plate as given in the table of section 6.10.2. Outflow conditions corresponding to the pressure $p = 101.3 \text{ kPa}$ at the outflow end of the computational domain were specified. No slip isothermal wall conditions are specified on the top and bottom plates with $T_{wall} = 320^\circ K$.

6.10.6 Results and Comparisons

The approximate analytical solution of the fully developed turbulent flow between parallel plates and the results obtained from the current study are given below and they are compared with each other.

Analytical solution of the fully developed flow between two parallel plates

The text by Arpaci and Larsen (1984) discusses the analytical solution of fully developed turbulent flow of an incompressible fluid between two parallel plates.

For steady and fully developed flow, $\partial/\partial t=0$ and $\partial u/\partial x=0$, where u is the mean velocity along the duct, and $\partial v/\partial y=0$ from the continuity equation. The linear momentum in x and y direction yield:

$$0 = -\frac{\partial p}{\partial x} + \frac{d}{dy}\left(\mu \frac{du}{dy} - \rho \bar{u}'v'\right) \quad (6.17)$$

$$0 = -\frac{\partial p}{\partial y} + \frac{d}{dy}(-\rho \bar{v}^2). \quad (6.18)$$

Integrating these equations, subject to the no slip condition at the top and bottom walls concludes (see Arpaci and Larsen (1984)):

$$u^+ = \int_0^{y^+} \frac{2(1 - y^+/2h^+) dy^+}{1 + \sqrt{1 + l^{+2}(1 - y^+/2h^+)}}, \quad (6.19)$$

where $h^+ = u_\tau h/\nu$; h is the space between the plates, $l^+ = u_\tau l/\nu = ky^+ D$; where D is the van Driest damping factor, $D = 1 - \exp(-\frac{y^+}{A^+})$ and $A^+ = 25$.

Very close to the wall, the molecular viscous effects are dominant and $\frac{y^+}{h^+/2} \ll 1$. Also $l^+ \rightarrow 0$ since $D \rightarrow 0$. In this region a typical value for y^+ is a value less than 5 and $h^+/2$ is about 1000 to 10,000. Therefore, $\frac{y^+}{h^+/2} \ll 1$ is a reasonable assumption. Hence in the close vicinity of the wall, Eqn. 6.19 is simplified and the viscous sub-layer formula is obtained as follows:

$$u^+ = y^+ \quad (6.20)$$

Moving out from the wall, still $\frac{y^+}{h^+/2} \ll 1$ and $D \rightarrow 1$ (hence $l^+ \rightarrow ky^+$). This yields the fully turbulent logarithmic law of the wall, i.e.

$$u^+ = \frac{1}{k} \ln y^+ + B \quad (6.21)$$

Various values for k and B are given in the literature. According to White (1991), the most appropriate values are $k = 0.41$ and $B = 5.0$.

The velocity profile obtained from the current computation is discussed next and will be compared to these analytical values given in the sub-layer and logarithmic regions (Eqns. 6.20 and 6.21) of the fully developed region.

Fully Developed Flow between Parallel Plates; Computations by the Current Study

Fig. 6.20 shows the velocity profile across the channel for four different cross sections $x=3.0, 4.0, 5.0$ and 6.0 meter, obtained with 151 grids along the channel and 51 in transverse direction. Fig 6.21 shows the same results obtained with a denser grid, i.e. 151×81 .

Fig. 6.22 shows the velocity profile obtained by analytical approximations as given by Eqns. 6.20 and 6.21 in the sub-layer and logarithmic regions and the velocity profile obtained by the current study with two grid densities. As shown in these figures the agreement is very good.

In the current computation the convergence is obtained by monitoring the mass flow rate across the duct. If the mass flow has remained relatively unchanged within 2000 iteration, then it is assumed that the flow has converged. It was found that there is a negligible mass deficit of about 0.044% from inlet plane to the exit plane, as shown in Fig. 6.23. This mass loss is due to the computational truncation error typical in any numerical study.

6.11 Conclusion

The formulation for the numerical flux based on the Roe scheme in generalized coordinates as outlined in Chapter 5 of this thesis (or Kermani and Plett (2001^b)), is applied to a very wide range of applications, and the results are compared with those of analytical solutions or experimental results. Good agreement for all the test cases has been obtained.

Figure 6.1: The schematic of inviscid fluxes entering and leaving the control volume in generalized coordinates.

Figure 6.2: Schematic of geometry for the laminar flow over a flat plate.

Figure 6.3: Grids for the flow over the flat plate; 31 grid along the plate and 21 across the plate with the clustering factor 1.7 near the bottom wall.

Figure 6.4: comparison of velocity profile for the flow over the flat plate.

Figure 6.5: Comparisons of skin friction along the plate.

Figure 6.6: Schematic of geometry for the laminar flow between two parallel plates. The dimension of the plate in the z direction is indicated by b , with $b \rightarrow \infty$.

Figure 6.7: Comparisons of pressure distribution between the two parallel plates.

Figure 6.8: Comparisons of velocity profile u between the two parallel plates.

Figure 6.9: Schematic of shock-wave interaction with laminar boundary layer on a flat plate.

Figure 6.10: The geometric configuration of the flow past the plate. In this figure, L is the location that incident shock impinges the plate if the flow were assumed inviscid.

Figure 6.11: Pressure distribution along the line $y \approx 0.01$ meter; pressure rise and pressure drop due to the leading edge shock, incident shock, compression wave, expansion fans and re-compression waves are shown here, obtained by current study.

Figure 6.12: Density contours; shock-wave interaction with laminar boundary layer on a flat plate, performed by current study.

Figure 6.13: A closer look at the separation bubble generated by a strong enough shock wave impinging on the boundary layer, as obtained by current study.

Figure 6.14: Pressure contour for the shock boundary layer interaction, obtained by current study on 201×201 grid.

Figure 6.15: Pressure contour for the shock impingement on the solid wall, obtained for inviscid flow by current study on 85×91 grid.

Figure 6.16: Comparison of pressure distribution on the wall for viscous and inviscid flow analysis, obtained by current study.

Figure 6.17: Comparison of computed pressure distribution over the wall with experimental values. The computation is performed in three grid densities.

Figure 6.18: Comparison of computed skin friction over the wall with experimental values. The computation is performed in three grid densities.

Figure 6.19: Grid configuration for the turbulent flow between two parallel plates. The enlarged picture of the duct is also shown in and around the inlet plane.

Figure 6.20: Turbulent flow velocity profile between two parallel plates in fully developed region, obtained with 151×51 grids.

Figure 6.21: Turbulent flow velocity profile between two parallel plates in fully developed region, obtained with 151×81 grids.

Figure 6.22: Comparisons of velocity profile for fully developed flow between two parallel plates, (i) obtained by analytical solution (see Arpaci and Larsen (1984)) and (ii) by the current computation in two different grid densities 151×51 and 151×81 . The prediction by the denser grid is in better agreement with the analytical solution than the one with the coarser mesh.

Figure 6.23: Mass flow rate along the channel at converged condition. Mass deficit is about 0.044%.

Chapter 7

Overall Conclusions

The main objective of this thesis was to develop a computer code (or a tool) to accurately solve the fluid equations. It was intended to discover any possible shortcomings of the numerical algorithms used for the problems addressed in this thesis, to modify or correct the captured shortcomings, and finally to assess the accuracy of the modified techniques. These objectives are itemized in Section 1.2 and it can be seen that these objectives have been very well met in this work. A brief summary is as follows.

Two major categories of Upwind Differencing (UD) algorithms, namely flux vector splitting (FVS) and flux difference splitting (FDS) are studied and modified and accuracy assessment of the modified formulae are performed over a wide range of test cases, from scalar Burgers' equation to two-dimensional flows governed by both Euler and Navier-Stokes equations.

Three different spatial discretization methods have been examined in this study as reported and documented in previous chapters. However, in the main chapter for the benchmarking purposes, Chapter 6, a third order upwind biased scheme with the van Albada flux limiter is used for the spatial discretization of convective and pressure terms. In this discretization, the primitive variables are extrapolated to the left and right faces of the cell by the MUSCL idea. For the temporal discretization, the second order two step predictor-corrector approach of the Lax-Wendroff family is used. The governing equations are recast into generalized coordinates in a simple and

novel form as described in Chapter 5 and are solved in this generalized coordinate system.

The method is applied to a variety of test cases ranging from the low subsonic regime (Mach number equal to 0.5) to supersonic flows (Mach number 4.0) for inviscid and viscous cases. Turbulence is modeled by the Baldwin and Lomax zero equation model. The mesh, which is structured, is developed either by an algebraic or orthogonal grid generator in a separate module and then transferred to the main solver. The versatility of applications used to verify the code gives enough confidence to permit the methods proposed in this study to be used in aerospace applications. However, as expected they are not free of shortcomings, which will be discussed in the section on possible opportunities for future research, as given in Section 7.2.

7.1 Summary of Contributions

A list of achievements and contributions resulting from this research is presented here, with the relative importance of each indicated by (*Major*) or (*minor*).

1. An entropy correction formula is developed and applied to the Roe scheme. This formula which is robust, i.e. needs no re-tuning, can be applied to a variety of PDE's ranging from the scalar Burgers equation, the shock tube problem, to multi-dimensional flow equations. This entropy fix formula is able to totally avoid expansion shocks in the sonic expansion regions without influencing the solution in the rest of the computational domain. (*Major*)
2. A second order non-oscillatory upwind scheme is developed by blending standard second and third order discretization of the inviscid fluxes each with an appropriate weight and applied to the van Leer scheme without implementing any flux limiter. The weighting factors are demonstrated to be universal with no adjusting needing to be applied to the factors for a variety of supersonic flows containing strong shock waves in planar coordinate systems. The aim for this part of the thesis was to show that it is possible to achieve a high resolution non-oscillatory scheme without implementation of a flux limiter. (*Major*)

3. The same issue as addressed in item number 2 has been successfully extended to axisymmetric flows containing strong shock waves, in which the same weighting factors as obtained for the above mentioned case are used and accurate results are obtained. (*minor*)
4. A formula is developed to give the numerical flux based on the Roe scheme in generalized coordinates. This formula is developed in a simple and novel way based on the flow parameters and grid-geometry. The accuracy of the formula is assessed by comparison with a variety of test cases. (*Major*)
5. The method as addressed in item number 4 is extended to viscous and turbulent flows and successfully applied to a variety of test cases. (*minor*)

7.2 Suggestions For Future Work

The following subjects are suggested as possible extensions of this research:

1. The numerical algorithm developed by blending the second and third order upwind schemes, as addressed in item number 2 in the previous section could be extended to a wider range of test cases with the objective of answering the following question: *are the weighting functions obtained the best values and to how wide range of aerospace applications can these weighting functions apply?*
2. The entropy correction formula developed and the numerical flux based on the Roe scheme in generalized coordinates has been extensively assessed and is ready to be applied to a range of engineering applications of aerospace. Moreover, the modifications are very simple and could easily be implemented in the numerical algorithms currently developed by others.
3. Higher order turbulence models could be added to the code in order to include the history of the flow field in modeling the turbulence rather than locally modeling the turbulence. Possibilities in this regard are: the Spalart and

Allmaras (1992) one equation model and the zonal two equation model of Menter (1993).

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Appendix A

Solutions of the Wave Equation

A.1 Introduction

The wave equation is a simple first order linear scalar equation given by:

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0, \quad (\text{A.1})$$

where a is a constant representing the wave speed. In this appendix two different types of solutions are sought for the wave equation, (i) physical solution and (ii) numerical solution. Once the numerical solution of the scalar wave equation is developed, the upwind differencing (UD) numerical techniques can be built into it based on the numerical solution of the wave equation. If a numerical scheme is developed for the wave equation, this provides enough confidence to use similar scheme to any other hyperbolic PDE in multi dimension (like Euler equations). For this reason, the wave equation is very suitable for the development of numerical schemes.

A.2 Physical Solution of the Wave Equation

For the physical solution of the wave equation, two types of solutions are obtained as follows:

Figure A.1: Schematic of the characteristic line C (with slope $dt/dx = 1/a$) in the x - t plane for the wave equation.

A.2.1 Physical Solution (# 1)

Eqn. A.1 is a hyperbolic equation with a as a constant. We consider the case of positive a . If a is negative, the problem is mirror-imaged.

To solve any hyperbolic equation an initial condition is required. For the wave equation, the initial condition is set to:

$$u(x, 0) = f(x), \quad (\text{A.2})$$

where $f(x)$ is the profile of u at initial time.

It can be proven that the general solution of the wave equation at any (x, t) has the form:

$$u(x, t) = f(x - at). \quad (\text{A.3})$$

The proof can be done by substituting Eqn. A.3 into the wave equation.

Using Eqn. A.3, for a given Δt one can write:

$$u(x, \Delta t) = f(x - a\Delta t) \quad (\text{A.4})$$

where Δt is the time elapsed from the time level n to $n + 1$, as shown in Fig. A.1.

Eqn. A.2 is valid for any arbitrary x including $x = x' - a\Delta t$. Therefore,

$$u(x' - a\Delta t, 0) = f(x' - a\Delta t). \quad (\text{A.5})$$

By a change of dummy variable:

$$u(x - a\Delta t, 0) = f(x - a\Delta t). \quad (\text{A.6})$$

The R.H.S. of Eqns. A.4 and A.6 are the same. Therefore,

$$u(x, \Delta t) = u(x - a\Delta t, 0) \quad (\text{A.7})$$

By considering Fig. A.1, the physical meaning of Eqn. A.7 is explained as follows. The solution at point B , i.e. $u(x, \Delta t)$, has exactly the same value at $a\Delta t$ upstream of x at previous time step, i.e. $u(x - a\Delta t, 0)$, as shown by point A . In other words:

$$u_B = u_A. \quad (\text{A.8})$$

A.2.2 Physical Solution (# 2)

The same type of solution for the wave equation could be given by more of a blend of the mathematical terminology as follows.

For u being a function of independent variables (x, t) , its differentiation could be determined by:

$$du = \frac{\partial u}{\partial t} dt + \frac{\partial u}{\partial x} dx \quad (\text{A.9})$$

giving the total derivative as:

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + \frac{dx}{dt} \frac{\partial u}{\partial x} \quad (\text{A.10})$$

If the magnitude of dx/dt is chosen in such a way that $dx/dt = a$, therefore, Eqn. A.10 becomes:

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} \quad (\text{A.11})$$

According to the wave equation, Eqn. A.1, the R.H.S. of Eqn. A.11 is zero. Therefore,

$$\frac{du}{dt} = 0, \quad (\text{A.12})$$

along $dx/dt = a$. It is noted that $du/dt = 0$ is only true if we move along a specific direction in the x - t plane, called a *characteristic direction*, the direction in which $dx/dt = a$ (see Fig. A.1). The line $dx/dt = a$ is called *characteristic line* and is denoted by C in Fig. A.1.

Eqns. A.8 and A.12 both represent a single concept, which is u satisfying

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0, \quad (\text{A.13})$$

or u remains constant (also said u is *invariant*) along the characteristic direction.

As shown in this section, the PDE of the wave equation given by Eqn. A.1 is reduced to the ODE (Eqn. A.12) along the characteristic direction. This is true for any hyperbolic PDE, which can be reduced to a corresponding ODE along the characteristic lines. The obtained ODE is called the *compatibility equation*.

A.3 Numerical Solution of the Wave Equation

Based on Eqns. A.8 or A.12, the numerical solution of the wave equation could be built. To achieve this goal u_A is needed to be determined (see Fig. A.1). An interpolation scheme is used between node j and its neighboring nodes to determine u_A . This interpolation scheme could be in any degree of accuracy. For example, a linear interpolation between nodes j and $j - 1$ at time level n gives:

$$\frac{u_j^n - u_A}{u_j^n - u_{j-1}^n} = \frac{a\Delta t}{\Delta x}. \quad (\text{A.14})$$

Therefore:

$$u_A = u_j^n - \frac{a\Delta t}{\Delta x} (u_j^n - u_{j-1}^n). \quad (\text{A.15})$$

According to Eqn. A.8, $u_B = u_A$. On the other hand, u_B is the solution of the wave equation at node j and at the new time step, i.e. time step $n + 1$. Therefore, the numerical solution of the wave equation at the new time step could be obtained as:

$$u_j^{n+1} = u_j^n - \frac{a\Delta t}{\Delta x} (u_j^n - u_{j-1}^n). \quad (\text{A.16})$$

This solution is developed based on the physical solution of the wave equation, as given by Eqns. A.8 or A.12. It relies on the fact that information propagates along

the characteristic direction, or on the fact that u is invariant along the characteristic direction, i.e. on the fact that the solution at u_A and u_B are equal.

A.4 Fundamentals of Upwind Differencing (UD)

Eqn. A.16, as the numerical solution of the wave equation, could be used to coin a variety of UD numerical algorithms. Usually upwind schemes are grouped into the following three major categories (see Manna (1992) for example):

1. Godunov type schemes,
2. Flux Vector Splitting (FVS) schemes, and
3. Flux Difference Splitting (FDS) schemes.

The Godunov type of schemes solve the governing equations by an iterative exact algorithm. They are sometimes referred to as exact Riemann solvers (ERS). For the scalar wave equation, the Godunov type of schemes are computationally efficient.

For a system of nonlinearly coupled equations like the fluid equations in multi-dimensions, ERS solves the equations in a locally one-dimensional frame of reference in each iteration and for each control volume. ERS basically assumes a localized shock tube problem for each control volume, in which exact solutions are sought at each iteration. Seeking the exact solution for multidimensional cases is not computationally efficient. So in this thesis, Godunov type of schemes, e.g. ERS, were not used. Hence no further explanation about these types of schemes will be given in this appendix.

For the rest of this appendix, Eqn. A.16 as the numerical solution of the wave equation, will be re-cast, or manipulated, into two different forms FVS and FDS, in which fundamentals of each of these upwind schemes are explained as these schemes are applied to the wave equation.

A.4.1 Basics of Flux Vector Splitting (FVS) Schemes

In this section, the numerical solution of the wave equation as given by Eqn. A.16, will be manipulated (or re-worded) and a form consistent with the FVS form of the wave equation is extracted. In other words, it will be shown that when the FVS scheme is applied to the wave equation, a numerical solution exactly equivalent to the Eqn. A.16 (for positive a 's) is obtained.

Manipulating (or Re-wording) Eqn. A.16

Considering Eqn. A.16 again, it can be seen that a first order forward difference in time is blended with a first order backward difference in space, i.e.

$$u_j^{n+1} = u_j^n - \frac{a\Delta t}{\Delta x} (u_j^n - u_{j-1}^n) \quad (\text{A.17})$$

where a is a positive scalar number (the wave speed). Positive a means the wave is moving in positive x direction. It is noted that the stability requirements of Eqn. A.17 demands backward spatial differencing for positive a , as the solution at a point is determined from its upstream condition. For negative a forward difference in space is required for the space discretization:

$$u_j^{n+1} = u_j^n - \frac{a\Delta t}{\Delta x} (u_{j+1}^n - u_j^n), \quad (\text{A.18})$$

otherwise the solution would be oscillatory.

A single equation could be given to cover both the negative and positive values of a (see Hirsch (1990) for example):

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} [a^+ (u_j^n - u_{j-1}^n) + a^- (u_{j+1}^n - u_j^n)] \quad (\text{A.19})$$

where a^+ is defined in such a way that it be equal to a for positive a , and zero for negative a . a^- is also defined in a similar way, i.e.

$$a^+ \equiv \max(a, 0) = \frac{1}{2} (a + |a|) \quad (\text{A.20})$$

$$a^- \equiv \min(a, 0) = \frac{1}{2} (a - |a|). \quad (\text{A.21})$$

Eqn. A.19 gives exactly the same result as Eqn. A.16 or Eqn. A.18 depending on the sign of a . On the other hand it can be shown that if the procedures for obtaining

the FVS schemes are adopted, an equation exactly similar to Eqn. A.19 would be obtained. These procedures are outlined below.

Flux Vector Splitting Scheme Applied to the Wave Equation

For a given hyperbolic PDE like the wave equation, the following procedures are taken to obtain the FVS form of the equation.

1. The governing equations are written in full conservative form. For the wave equation

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0, \quad (\text{A.22})$$

where $f = au$ is the scalar advective flux.

2. The Jacobian of f is obtained as: $\partial f / \partial u = a$.
3. The following form of space discretization is finally applied depending on the sign of a , (i) backward difference for the positive a 's, that is because information is received from upstream and (ii) forward difference for the negative a 's, that is because information is received from downstream.

Steps 1 to 3 are performed to discretize any hyperbolic equation by FVS schemes. When, these steps are applied to the scalar wave equation an equation equivalent to Eqn. A.19 is obtained. In other words, Eqn. A.19 is the numerical discretization of the wave equation by FVS schemes. On the other hand Eqn. A.19 is a single equation, which represents the numerical solution of the wave equation for both positive and negative a 's. This shows that the wave equation is a very useful and helpful equation, which allows the UD numerical schemes to be coined based on its numerical solution.

A.4.2 Basics of Flux Difference Splitting (FDS) Schemes

In section A.4.1 two equations A.17 and A.18 were firstly given as the numerical solution of the wave equation, one for the positive values of a and the other for the negative values of a . The Eqns. A.17 and A.18 were reduced to a single equation

Figure A.2: Numerical fluxes f_E and f_W passing east and west faces of the cell j .

namely, Eqn. A.19, and it was later shown that Eqn. A.19 is also the numerical discretized form of the wave equation by FVS schemes.

In this section the wave equation will be re-cast into another form, which is equivalent to the FDS discretization of the wave equation.

Eqns. A.17 and A.18 are reduced to another form, as follows:

$$u_j^{n+1} = u_j^n - \frac{a\Delta t}{2\Delta x} [u_{j+1}^n - u_{j-1}^n] + \frac{\Delta t}{2\Delta x} |a| [u_{j+1}^n - 2u_j^n + u_{j-1}^n]. \quad (\text{A.23})$$

For positive a 's, $|a| = a$, and Eqn. A.23 is simplified to Eqn. A.17 and for negative a 's, $|a| = -a$, and Eqn. A.23 is simplified to Eqn. A.18. Eqn. A.23 looks like a second order CD approach in space, with an artificial diffusion added. But in fact it is an upwind differencing algorithm, as mentioned earlier it is equivalent to the wave equation.

In the following, the discretized form of the wave equation by FDS schemes is obtained and it is shown that an equation exactly equivalent to Eqn. A.23 is the result.

Flux Difference Splitting Scheme Applied to the Wave Equation

The following procedures are taken to discretize the wave equation by the FDS scheme:

1. The wave equation is written in full conservative form as:

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0, \quad (\text{A.24})$$

Then, the numerical solution of the wave equation can be written in a quasi central-difference as:

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} (f_E - f_W) \quad (\text{A.25})$$

where f_E and f_W are the numerical fluxes at the east and the west faces of cell j , as shown by Fig. A.2.

2. The numerical fluxes f_E and f_W are obtained by equating Eqns. A.23 and A.25 term by term. Recalling that $f = a u$:

$$f_E = \frac{1}{2} [f_j^n + f_{j+1}^n] - \frac{1}{2} |a| (u_{j+1}^n - u_j^n) \quad (\text{A.26})$$

and f_W as:

$$f_W = \frac{1}{2} [f_{j-1}^n + f_j^n] - \frac{1}{2} |a| (u_j^n - u_{j-1}^n). \quad (\text{A.27})$$

Eqn. A.25 together with the numerical fluxes f_E and f_W is the discretized form of the wave equation by FDS schemes.

The discretization of fluid equations by FVS and FDS schemes are given in Appendix B.

A.4.3 Exact vs. Approximate Riemann Solvers

As mentioned in section A.4, ERS are not computationally efficient for the multi-dimensional fluid equations. Alternatively, Approximate Riemann Solver (ARS) schemes are used to solve the fluid equations by iterative methods. ARS solve the linearized form of the fluid equations, which are computationally efficient and at the same time they are accurate. On the other hand, there is a penalty. That is the entropy conditions are not satisfied, as the expansion shocks (physically impossible phenomena in nature) are valid solutions of the linearized equations, therefore, expansion shocks are captured in the same way as the shock waves are captured. This deficiency is fixed by an entropy correction technique as outlined in chapter 4.

One of the most popular ARS schemes, is the FDS scheme of Roe (1981). More details of the Roe's FDS scheme are given in Appendix D.

A.4.4 Numerical Flux f_E ; Agreement with UD

Eqn. A.25 as the discretized form of the wave equation by an FDS scheme is shown in a form of a quasi-central difference scheme. In this section the numerical flux f_E , given by Eqn. A.26, is examined to see whether it agrees with the essence of UD. f_E by a first order UD scheme reduces to: (see Fig. A.2)

$$f_E = \begin{cases} \frac{1}{2} [au_j^n + au_{j+1}^n] - \frac{1}{2}(a)(u_{j+1}^n - u_j^n) = au_j^n & a > 0 \\ \frac{1}{2} [au_j^n + au_{j+1}^n] - \frac{1}{2}(-a)(u_{j+1}^n - u_j^n) = au_{j+1}^n & a < 0, \end{cases} \quad (\text{A.28})$$

For positive values of a , f_E is determined from its upstream value, i.e. au_j^n , and for negative values of a , f_E is determined from its downstream value, i.e. au_{j+1}^n . This totally agrees with the essence of upwind schemes.

A.4.5 Stability Criteria of the FVS and FDS Schemes

The stability criterion of the FVS and FDS numerical schemes as applied to the scalar wave equation is given here. It can be shown that the stability criterion for all the numerical schemes introduced in this section, is the standard CFL condition, see Tannehill et. al (1997). That is:

$$\frac{\Delta t}{\Delta x} |u_{max}| \leq 1. \quad (\text{A.29})$$

A.5 Conclusion

The highlights of derivations of this appendix are:

1. The physical solution of the wave equation considers the side from which the disturbances are propagating (the speed of propagation is the wave speed). As the numerical solution of the wave equation has been built in a way totally consistent with its physical solution, therefore, it takes into account the side from which the information is flowing.

2. The numerical solution of the wave equation could be tailored (or manipulated or re-worded) in such a way that it is equivalent to the discretized form of the wave equation by FVS and FDS schemes.
3. The discretization of the wave equation by FVS and FDS schemes give exactly the same values, both being equivalent to the numerical solution of the wave equation. However, the discretization of the fluid equation by FVS and FDS schemes are different. The difference between FVS and FDS when applied to the fluid equations are explained in Appendices B and C.
4. Finally, in this appendix it is observed that the wave equation is very useful equation which allows the fundamentals of upwind schemes to be demonstrated based on its numerical solution.

Appendix B

Solution of the Characteristic Form of the Fluid Equations

B.1 Introduction

In Appendix A the PDE of the wave equation was reduced to an ODE along its characteristic line and later the fundamental equations of two major categories of UD schemes, FVS and FDS, were developed.

The extension of this method to fluid equations is performed in this Appendix and Appendix C. The current appendix, Appendix B, has two parts:

1. Part I; the decomposition of fluid equations, in which the fluid equations for one-dimensional flow, as given by Eqn. 2.5, are decomposed into a form similar to that of the wave equation, i.e. into a form similar to Eqn. A.1.
2. Part II; the solution of the decomposed equations, in which the obtained decomposed equations in Part I are solved in the same way that the wave equations are solved and the same results as for the wave equations, as given by Eqns. A.8 or A.12, are obtained. Riemann invariants and the basis of the Method of Characteristics are also explained in this part.

The formulations for the solution of fluid equations by FVS and FDS schemes are given in Appendix C.

B.2 Part I; Decomposition of Fluid Equation

Consider the fluid equations in vector form, as given by Eqn. 2.5 for the one-dimensional flow, which is also repeated here:

$$\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} = 0. \quad (\text{B.1})$$

For the one dimensional flow, the vector Eqn. B.1 represents three scalar equations continuity, momentum and energy, where Q is the solution vector and F is the flux vector. These equations are strongly coupled and are impossible to solve independently. To develop a solution for the fluid equation, similar to the solution which was obtained for the wave equation in Appendix A, Eqn. B.1 is needed to be decomposed into a set of un-coupled equations (three equations for the one-dimensional flow). The decomposition of Eqn. B.1 is possible as Eqn. B.1 is a hyperbolic PDE (hyperbolic equations could be reduced to ODE's along the characteristic lines). Once the decomposition is completed, a set of un-coupled equations are obtained in so called *characteristic form*.

B.2.1 Converting Fluid Equations into Quasi-Linear Form

To decompose the fluid equations, Eqn. B.1, it is first required to write these equations in a quasi-linear form, as:

$$\frac{\partial Q}{\partial t} + [A] \frac{\partial Q}{\partial x} = 0 \quad (\text{B.2})$$

where $[A]$ is the Jacobian matrix of the flux F , given by:

$$[A] \equiv \frac{\partial F}{\partial Q}. \quad (\text{B.3})$$

Jacobian matrix $[A]$, a 3×3 matrix for the one-dimensional flow, is:

$$[A] \equiv \begin{bmatrix} \frac{\partial f_1}{\partial q_1} & \frac{\partial f_1}{\partial q_2} & \frac{\partial f_1}{\partial q_3} \\ \frac{\partial f_2}{\partial q_1} & \frac{\partial f_2}{\partial q_2} & \frac{\partial f_2}{\partial q_3} \\ \frac{\partial f_3}{\partial q_1} & \frac{\partial f_3}{\partial q_2} & \frac{\partial f_3}{\partial q_3} \end{bmatrix} \quad (\text{B.4})$$

where

$$Q \equiv \begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix} \equiv \begin{bmatrix} \rho \\ \rho u \\ \rho e_t \end{bmatrix}, \quad F \equiv \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} \equiv \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (\rho e_t + p)u \end{bmatrix}. \quad (\text{B.5})$$

To calculate $[A]$, it is necessary to write F in terms of the components of Q , i.e.

$$F = \begin{bmatrix} q_2 \\ \frac{q_2^2}{q_1} + (\gamma - 1)\left[q_3 - \frac{1}{2}\frac{q_2^2}{q_1}\right] \\ \left[\gamma q_3 - \frac{\gamma-1}{2}\frac{q_2^2}{q_1}\right] \frac{q_2}{q_1} \end{bmatrix}, \quad (\text{B.6})$$

then differentiate each element of F w.r.t. Q according to Eqn. B.4. This task has been done by software Maple, version V release 5, as an excellent source for symbolic work, and $[A]$ is determined. This is shown at the end of this Appendix, and repeated here for convenience:

$$[A] = \begin{bmatrix} 0 & 1 & 0 \\ -\frac{1}{2}(3-\gamma)u^2 & (3-\gamma)u & (\gamma-1) \\ -\frac{c^2 u}{\gamma-1} - \frac{2-\gamma}{2}u^3 & \frac{3-2\gamma}{2}u^2 + \frac{c^2}{\gamma-1} & \gamma u \end{bmatrix}. \quad (\text{B.7})$$

- **Definition:** For a given F as a function of components of Q , like Eqn. B.6, and an arbitrary number s , if :

$$F(sQ) = s^p F(Q), \quad (\text{B.8})$$

then F is said to be a *homogenous function* of degree p w.r.t. Q .

F , given by Eqn. B.6, has this remarkable property of being the homogenous function of degree $p=1$ of the components of Q . This is a very important property for F , which allows the following equation to be valid:

$$F(Q) = [A] Q \quad (\text{B.9})$$

The Maple software is again used to prove Eqn. B.9, i.e. $F(Q) = [A] Q$. The proof of Eqn. B.9 in general form, for an m element vector, could be found for example, in the CFD lecture notes of MacCormack(1995).

B.2.2 Eigenvalues and Eigenvectors of the Jacobian Matrix

As another intermediate step in obtaining the decomposed form of the fluid equations, the eigenvalues of $[A]$, are needed. Mathematically eigenvalues of square matrix $[A]$ are defined as follows.

$[A]$ is considered as a transformation matrix in the vectorial x space that is applied to a general vector T , or better to say multiplied by T , and the resultant vector b is produced, i.e. $[A]T = b$. In the eigenvalue problem, we are looking for specific directions T if the transformation matrix $[A]$ is applied to them, the resultant b stays along T , i.e. T and b lie in the same direction. In other words, $b = \lambda T$, where λ is a scalar number, namely an eigenvalue of $[A]$. Therefore, one can write:

$$[A]T = \lambda T \quad (\text{B.10})$$

or equivalently,

$$([A] - \lambda I)T = 0 \quad (\text{B.11})$$

where I is the unit matrix. To obtain non-zero values of T the determinant of its coefficients must vanish, where an equation so called *characteristic equation*, is determined:

$$\det([A] - \lambda I) = 0. \quad (\text{B.12})$$

λ 's, the eigenvalues of $[A]$, are determined from the characteristic equation, i.e. Eqn. B.12. $[A]$ contains three eigenvalues as it is a 3×3 matrix for a one-dimensional fluid equations. These eigenvalues have been determined again by Maple and repeated here (see the end of this Appendix),

$$\lambda_1 = u \quad \lambda_2 = u + c \quad \lambda_3 = u - c \quad (\text{B.13})$$

where c is the speed of sound given by: $c = \sqrt{\gamma \frac{p}{\rho}}$. As seen from Eqn. B.13 the eigenvalues of $[A]$ are all real. For a hyperbolic PDE, it can be shown that all eigenvalues are real. The corresponding eigenvectors are also determined by Maple,

(see the end of this Appendix). They are:

$$T^{(1)} = \begin{bmatrix} 1 \\ u \\ \frac{u^2}{2} \end{bmatrix},$$

$$T^{(2)} = \begin{bmatrix} 1 \\ u + c \\ \frac{1}{2}u^2 + \frac{c^2}{\gamma-1} + uc \end{bmatrix}, \quad T^{(3)} = \begin{bmatrix} 1 \\ u - c \\ \frac{1}{2}u^2 + \frac{c^2}{\gamma-1} - uc \end{bmatrix}. \quad (\text{B.14})$$

- **Theorem:** It can be shown that for any non-zero and arbitrary number α , if $T^{(1)}$ is an eigenvector, therefore, $\alpha T^{(1)}$ will also be an eigenvector. The proof of this is straight-forward simply by substituting the new eigenvectors, $\alpha T^{(1)}$, into Eqn. B.10.

In this theorem, α is called the *normalization factor*. Choosing the normalization factors $\alpha = 1$, $\beta = \delta = \frac{\rho}{2c}$, as often found in the literature, (see for example Hirsch(1990) or Hoffmann and Chiang(1993)), also recalling that $\frac{1}{2}u^2 + \frac{c^2}{\gamma-1} = H$, where H is the stagnation enthalpy, therefore, another set of eigenvectors are introduced as:

$$T^{(1)} = \begin{bmatrix} 1 \\ u \\ \frac{u^2}{2} \end{bmatrix}, \quad T^{(2)} = \begin{bmatrix} 1 \\ u + c \\ H + uc \end{bmatrix} \frac{\rho}{2c}, \quad T^{(3)} = \begin{bmatrix} 1 \\ u - c \\ H - uc \end{bmatrix} \frac{\rho}{2c}. \quad (\text{B.15})$$

The choice of normalization factors does not change the type of problem. However, they should be chosen in a way appropriate to the flow field. For example, $\alpha = \frac{1}{u}$ is also a normalization factor. But it is not an appropriate choice as it causes problems in the vicinity of stagnation points.

B.2.3 Diagonalization of the Jacobian Matrix

To obtain the decomposed form of the fluid equations, it is necessary to diagonalize the Jacobian matrix $[A]$. That is:

$$[A] = [T] [\Lambda] [T]^{-1} \quad (\text{B.16})$$

where $[\Lambda]$ is the diagonal matrix of the eigenvalues, that is why this section is called diagonalization of the Jacobian matrix, i.e.

$$[\Lambda] = \begin{bmatrix} u & 0 & 0 \\ 0 & u + c & 0 \\ 0 & 0 & u - c \end{bmatrix}, \quad (\text{B.17})$$

$[T]$ is the eigenvector matrix, determined in a way that each eigenvector is accommodated in each column of $[T]$, i.e.

$$[T] = \begin{bmatrix} 1 & \frac{\rho}{2c} & \frac{\rho}{2c} \\ u & (u + c)\frac{\rho}{2c} & (u - c)\frac{\rho}{2c} \\ \frac{u^2}{2} & (H + uc)\frac{\rho}{2c} & (H - uc)\frac{\rho}{2c} \end{bmatrix}, \quad (\text{B.18})$$

and $[T]^{-1}$ is the inverse of $[T]$, determined by Maple, as given at the end of this Appendix:

$$[T]^{-1} = \begin{bmatrix} \frac{-u^2 + u^2\gamma - 2c^2}{-2c^2} & \frac{u(\gamma - 1)}{c^2} & -\frac{\gamma - 1}{c^2} \\ \frac{u(-u - 2c + \gamma u)}{2\rho c} & \frac{u + c - \gamma u}{\rho c} & \frac{\gamma - 1}{\rho c} \\ \frac{u(-u + 2c + \gamma u)}{2\rho c} & \frac{-u + c + \gamma u}{\rho c} & -\frac{\gamma - 1}{\rho c} \end{bmatrix}. \quad (\text{B.19})$$

The way that the eigenvalue and the eigenvector matrices are arranged should be noted. That is, if the eigenvalue λ_1 appears in the first row of $[\Lambda]$, then its corresponding eigenvector, i.e. $T^{(1)}$, should appear in the first column of $[T]$. The same procedure is extended to all of the eigenvalues and eigenvectors.

B.2.4 Decomposed Form of the Fluid Equations

After the fluid equations are written in quasi-linear form (Section B.2.1), the eigenvalues and eigenvectors of the Jacobian matrix are determined (Section B.2.2), and the Jacobian matrix is diagonalized (Section B.2.3), the decomposition of the fluid equations is straight forward. The decomposition of the fluid equation is performed in this section as follows.

Eqn. B.16 is substituted into Eqn. B.2. Therefore,

$$\frac{\partial Q}{\partial t} + [T][\Lambda][T]^{-1} \frac{\partial Q}{\partial x} = 0. \quad (\text{B.20})$$

By multiplying $[T]^{-1}$ to Eqn. B.20:

$$[T]^{-1} \frac{\partial Q}{\partial t} + [T]^{-1} [T] [\Lambda] [T]^{-1} \frac{\partial Q}{\partial x} = 0. \quad (\text{B.21})$$

For Q as the solution vector, its differentiation could be determined as:

$$\delta Q = \begin{bmatrix} \delta \rho \\ \rho \delta u + u \delta \rho \\ \frac{\delta p}{\gamma - 1} + \frac{1}{2} u^2 \delta \rho + \rho u \delta u \end{bmatrix}, \quad (\text{B.22})$$

and a parameter the so called *wave amplitude vector* is defined as follows:

$$\delta W \equiv [T]^{-1} \delta Q. \quad (\text{B.23})$$

δW is calculated again by our tool for symbolic algebraic work, Maple, and is shown at the end of this Appendix, also repeated here for convenience:

$$\delta W \equiv \begin{bmatrix} \delta w_1 \\ \delta w_2 \\ \delta w_3 \end{bmatrix} = \begin{bmatrix} \delta \rho - \frac{\delta p}{c^2} \\ \delta u + \frac{\delta p}{\rho c} \\ -\delta u + \frac{\delta p}{\rho c} \end{bmatrix}. \quad (\text{B.24})$$

Therefore, Eqn. B.21 reduces to:

$$\frac{\partial W}{\partial t} + [\Lambda] \frac{\partial W}{\partial x} = 0. \quad (\text{B.25})$$

Eqn. B.25 is the equation that we have been trying to obtain by gradual progress from Section B.2.1 until here. It is in fact a converted form of the fluid equation in the so called *decomposed form*, also called *characteristic form*. Eqn. B.25 is in vector form and suggests three scalar equations:

$$\begin{aligned} \frac{\partial w_1}{\partial t} + \lambda_1 \frac{\partial w_1}{\partial x} &= 0 \\ \frac{\partial w_2}{\partial t} + \lambda_2 \frac{\partial w_2}{\partial x} &= 0 \\ \frac{\partial w_3}{\partial t} + \lambda_3 \frac{\partial w_3}{\partial x} &= 0. \end{aligned} \quad (\text{B.26})$$

These equations are un-coupled as opposed to the original form of the fluid equations, Eqn. B.1, which were strongly coupled.

Solution of the decomposed equations of fluid motion is given in Appendix C.

B.3 Part II; Solution of the Decomposed Equations

The converted fluid equations to the so called decomposed form of the fluid equations, Eqns. B.26, are similar in form to the wave equation, i.e. Eqn. A.1, allowing Eqns. B.26 to be treated in the same way that the scalar wave equation was treated. That is, a very similar strategy as for the wave equation could be taken to solve Eqns. B.26.

Before obtaining the solution of Eqns. B.26, it may be appropriate to review what has been discussed to the is point in this Appendix. The non-linear equations of fluid motion have been recast into a form similar to that of the wave equation, namely the characteristic form given by Eqns. B.26.

Also recalling from Appendix A, the wave equation in which u is an invariant along the characteristic direction $dx/dt = a$, safely along which information is allowed to propagate. The same concept is extended to Eqns. B.26, where w_1 , w_2 , and w_3 do not vary along the directions $dx/dt = \lambda_1$, $dx/dt = \lambda_2$, and $dx/dt = \lambda_3$, respectively, (see Fig. B.1). The parameters w_1 , w_2 , and w_3 are called *Riemann invariants*, the parameters which are constant along the characteristic lines. The magnitude of these constants will be obtained based on the flow properties. It is also noted that similar to the wave equation, in Eqns. B.26, λ 's, the eigenvalues of $[A]$, are equivalent to the wave speed, a in Eqn. A.1.

Considering one of the equations B.26, the quantity w satisfying:

$$\frac{\partial w}{\partial t} + \lambda \frac{\partial w}{\partial x} = 0 \quad (\text{B.27})$$

is constant along the characteristic line C defined by $dx/dt = \lambda$, because along C , the total derivative dw/dt vanishes. That is:

$$\frac{dw}{dt} \equiv \frac{\partial w}{\partial t} + \frac{dx}{dt} \frac{\partial w}{\partial x} = 0, \quad (\text{B.28})$$

or equivalent to Eqn. A.12, one can write:

$$\frac{dw}{dt} = 0. \quad (\text{B.29})$$

Figure B.1: C^0 , C^- , and C^+ characteristic lines for a one-dimensional inviscid flow.

For each w along its own characteristic line, it could be written: (see Fig. B.1):

$$\begin{array}{llll}
 w_1 = \text{constant} & \text{along} & C^0 : & \frac{dx}{dt} = u, \\
 w_2 = \text{constant} & \text{along} & C^+ : & \frac{dx}{dt} = u + a, \\
 w_3 = \text{constant} & \text{along} & C^- : & \frac{dx}{dt} = u - a.
 \end{array} \quad (\text{B.30})$$

In the next section, Section B.3.1, Riemann invariants (w_1 , w_2 , and w_3), will be determined in terms of fluid properties, and the basis of the Method of Characteristics will be explained in Section B.3.2.

B.3.1 Riemann Invariants

Suppose at a point in the x - t plane, w_1 , w_2 , and w_3 are given, and it is required to determine the primitive variables of the fluid, i.e. ρ , p , and u at this point. To do so, the relations between w 's and the primitive variables of the fluid are needed. In Section B.3, in Eqns. B.30, it is found that w 's are constant along the characteristic lines. In this section the magnitude of these constants, i.e. Riemann invariants, are

determined in terms of fluid primitive variables. Combining Eqns. B.24 and B.29 concludes that,

$$d\rho - \frac{dp}{c^2} = 0, \quad \text{along} \quad \frac{dx}{dt} = u \quad (\text{B.31})$$

$$du + \frac{dp}{\rho c} = 0, \quad \text{along} \quad \frac{dx}{dt} = u + c \quad (\text{B.32})$$

$$-du + \frac{dp}{\rho c} = 0, \quad \text{along} \quad \frac{dx}{dt} = u - c. \quad (\text{B.33})$$

As for the wave equation, the PDE's B.26 are reduced to the ODE's B.31 to B.33 along the characteristic lines.

In order to determine the Riemann invariants w_1 , w_2 , and w_3 , Eqns. B.31 to B.33 are integrated as follows:

Entropy Wave

Consider Eqn. B.31 and multiply it by $-\gamma c_v/\rho$, where γ is the ratio of the specific heats and c_v is the constant volume specific heat. That gives:

$$-\frac{\gamma c_v}{\rho} \left(d\rho - \frac{dp}{c^2} \right) = 0 \quad \text{along} \quad \frac{dx}{dt} = u. \quad (\text{B.34})$$

On the other hand, it can be shown that:

$$ds = -\frac{\gamma c_v}{\rho} \left(d\rho - \frac{dp}{c^2} \right), \quad (\text{B.35})$$

where s is the specific entropy. Hence,

$$ds = 0 \quad \text{along} \quad \frac{dx}{dt} = u. \quad (\text{B.36})$$

That is, entropy remains constant along C^0 (see Fig. B.1). For this reason Eqn. B.31 is referred to as the *entropy wave equation*. It is therefore concluded that $w_1 = \text{constant}$ along $dx/dt = u$ is equivalent to $s = \text{constant}$ along this line, i.e. the characteristic line C^0 indicates an isentropic process line.

First- and Second-Acoustic Waves

Eqns. B.32 and B.33 are also integrated for isentropic flow, in which $p/\rho^\gamma = \text{constant}$, along the characteristic lines C^+ and C^- . This results:

$$w_2 = \frac{2}{\gamma - 1} c + u \quad (\text{B.37})$$

$$w_3 = \frac{2}{\gamma - 1}c - u. \quad (\text{B.38})$$

B.3.2 Basis of the Method of Characteristics

Solution of the characteristic form, or decomposed form, of the fluid equations will be obtained in this section, after which the Riemann invariants are determined. What is referred to as the solution of the decomposed form of the fluid equation is that w 's in the new time level are determined. Therefore, the primitive variables ρ , p and u are determined via Eqns. B.36 to B.38.

This approach is the direct application of what has been obtained to this point, and the method is the basis of the *Method of Characteristics*.

Consider Fig. B.2 and suppose at time level n all the primitive variables, ρ , p and u are known at all nodes j , $j + 1$, etc. These primitive variables are denoted by ρ_j^n , p_j^n and u_j^n . It is desired to determine all of these primitive variables at time level $n + 1$, i.e. ρ_j^{n+1} , p_j^{n+1} and u_j^{n+1} .

According to the numerical solution of the wave equation, say Eqn. A.19, the Riemann invariants w_2 and w_3 at the new time level are determined from:

$$w_{2,j}^{n+1} = w_{2,j}^n - \frac{\Delta t}{\Delta x} \left[\lambda_2^+ (w_{2,j}^n - w_{2,j-1}^n) + \lambda_2^- (w_{2,j+1}^n - w_{2,j}^n) \right]. \quad (\text{B.39})$$

$$w_{3,j}^{n+1} = w_{3,j}^n - \frac{\Delta t}{\Delta x} \left[\lambda_3^+ (w_{3,j}^n - w_{3,j-1}^n) + \lambda_3^- (w_{3,j+1}^n - w_{3,j}^n) \right]. \quad (\text{B.40})$$

That is, $w_{2,j}^{n+1}$ and $w_{3,j}^{n+1}$ are determined at point B as shown in Fig. B.2 (it is noted that another type of solution for the decomposed form of the fluid equations could also be obtained if a solution similar to Eqn. A.23 is written for the decomposed form of fluid equations).

The obtained values $w_{2,j}^{n+1}$ and $w_{3,j}^{n+1}$ from Eqns. B.39 and B.40 may then be used to determine u_j^{n+1} and c_j^{n+1} if Eqns. B.37 and B.38 are used. That is:

$$u_j^{n+1} = \frac{w_{2,j}^{n+1} - w_{3,j}^{n+1}}{2}, \quad (\text{B.41})$$

$$c_j^{n+1} = \frac{w_{2,j}^{n+1} + w_{3,j}^{n+1}}{2}(\gamma - 1). \quad (\text{B.42})$$

The pressure and density at the new time level are obtained as follows. Pressure.

Figure B.2: Three characteristic lines C^0 , C^+ , and C^- configuration for one-dimensional subsonic flow. Region A^+ to A^- is the domain which influences the solution at point B .

density and speed of sound are related through:

$$c_j^{n+1} = \sqrt{\gamma \frac{p_j^{n+1}}{\rho_j^{n+1}}} \quad (\text{B.43})$$

Also from Eqn. B.36, where the isentropic relation is implied along the characteristic line C^0 ($dx/dt = u$), one can write:

$$\frac{p}{\rho^\gamma} = \text{constant} \equiv K = \frac{p_j^{n+1}}{(\rho_j^{n+1})^\gamma}, \quad \text{along} \quad \frac{dx}{dt} = u. \quad (\text{B.44})$$

That is, K is not varying along the characteristic line C^0 . It should be noted that all the quantities $K=\text{constant}$, $w_1=\text{constant}$, or $s=\text{constant}$ correspond to a single isentropic process shown by C^0 in Fig. B.2. As a result, according to Eqn. A.19, for the invariant quantity K along C^0 , it can be written:

$$K_j^{n+1} = K_j^n - \frac{\Delta t}{\Delta x} \left[\lambda_1^+ (K_j^n - K_{j-1}^n) + \lambda_1^- (K_{j+1}^n - K_j^n) \right]. \quad (\text{B.45})$$

Knowing K_j^{n+1} , the two unknowns ρ_j^{n+1} and p_j^{n+1} could be determined from the two Eqns. B.43 and B.44. That is, all the parameters ρ_j^{n+1} , p_j^{n+1} and u_j^{n+1} are determined, Q.E.D. This procedure can be extended to all j 's at each new time step for which appropriate boundary conditions are imposed. That is, all the flow primitive variables are obtained at any new time step at all nodes.

This approach is the direct solution of the characteristic form of the fluid equations. It is the basis of the method of characteristics. This approach has some implementation difficulties when it is extended to multidimensional flows as the locations of nodes are not independently chosen. This becomes more complicated as the method is applied to unsteady compressible flows. Moreover, in this approach at each time step the flow primitive variables should be determined from the Riemann invariants, which results in excessive computational costs. Another approach, which is still based on the numerical solution of the decomposed form of fluid equations (or the wave equations) and is more easily applied to for multidimensional unsteady CFD applications, is needed. This approach is addressed in Appendix C.

B.4 Formulae Derivations by Maple

The formulae derivations by Maple, is given in the next page.

```

> restart;
> # (1) INTRODUCING THE FLUX VECTOR "F" AS A FUNCTION OF "Q":
> F1:=q2: F1:=simplify(%):
> F2 := q2^2/q1 + (gamma-1)*( q3-1/2*(q2^2/q1) ): F2:=simplify(%):
> F3:=( gamma*q3- (gamma-1)/2*(q2^2/q1) )*q2/q1: F3:=simplify(%):
> F:=array([ [F1],[F2],[F3] ]);

```

$$F := \begin{bmatrix} \frac{q^2}{2} \frac{1}{q^1} \frac{3 q^2 + 2 \gamma q^3 q^1 - \gamma q^2 - 2 q^3 q^1}{q^1} \\ \frac{1}{2} \frac{(2 \gamma q^3 q^1 - \gamma q^2 + q^2) q^2}{q^1^2} \end{bmatrix}$$

```

> #
> # (2) FLUX JACOBIAN "A" IS OBTAINED BY DIFFERENTIATING "F" W.R.T
> "Q", I.E. A=DF/DQ:
> a11:=diff(F1,q1): a12:=diff(F1,q2): a13:=diff(F1,q3):
> a21:=diff(F2,q1): a22:=diff(F2,q2): a23:=diff(F2,q3):
> a31:=diff(F3,q1): a32:=diff(F3,q2): a33:=diff(F3,q3):
> A:=array([ [a11,a12,a13],[a21,a22,a23],[a31,a32,a33] ]): A:=simplify(%);

```

$$A := \begin{bmatrix} 0 & 1 & 0 \\ \frac{1}{2} \frac{q^2 (-3 + \gamma)}{q^1^2} & -\frac{q^2 (-3 + \gamma)}{q^1} & \gamma - 1 \\ -\frac{q^2 (\gamma q^3 q^1 - \gamma q^2 + q^2)}{q^1^3} & \frac{1}{2} \frac{-3 \gamma q^2 + 3 q^2 + 2 \gamma q^3 q^1}{q^1^2} & \frac{\gamma q^2}{q^1} \end{bmatrix}$$

```

> #
> # (3) SUBSTITUTING THE VALUES FOR "q":
> q1:=rho: q2:=rho*u: q3:=rho*c^2/gamma/(gamma-1) + 1/2*rho*u^2:
> Q:=array([ [q1],[q2],[q3] ]);

```

$$Q := \begin{bmatrix} \rho \\ \rho u \\ \frac{\rho c^2}{\gamma(\gamma-1)} + \frac{1}{2} \rho u^2 \end{bmatrix}$$

```

> # (4) VERIFY THE HOMOGENIOUS PROPERTY OF "F" AS A FUNCTION OF
> "Q" BY MULTIPLYING "A . Q" TO SEE IF IT RECEOVERS "F":
> with(linalg): multiply(A,Q): F:=simplify(%);

```

Warning, new definition for norm

Warning, new definition for trace

$$F := \begin{bmatrix} \frac{\rho u}{\gamma} \\ \frac{(u^2 \gamma + c^2) \rho}{\gamma} \\ \frac{1}{2} \frac{u \rho (2c^2 + u^2 \gamma - u^2)}{\gamma - 1} \end{bmatrix}$$

```
> #
> # (5) OBTAIN EIGENVALUES OF "A" & THE CORESPONDING EIGENVECTORS:
> lambda:=eigenvals(A); eigenvectors(A);
      λ := u, u + c, u - c
```

$$\left[u, 1, \left\{ \left[\frac{1}{u}, 1, \frac{1}{2} u \right] \right\}, [u + c, 1, \left\{ \left[1, u + c, \frac{1}{2} \frac{-u^2 + u^2 \gamma - 2cu + 2c^2 + 2\gamma u c}{\gamma - 1} \right] \right\}], \right. \\ \left. [u - c, 1, \left\{ \left[1, u - c, -\frac{1}{2} \frac{u^2 - u^2 \gamma - 2cu - 2c^2 + 2\gamma u c}{\gamma - 1} \right] \right\}] \right]$$

```
> #
> # (6) DEVELOPE THE EIGENVECTOR MATRIX:
> H:=1/2*u^2+c^2/(gamma-1): # Definition of Total Enthalpy
> T11:=1: T21:=u: T31:=u^2/2:
> T12:=1*rho/(2)/c: T22:=(u+c)*rho/(2)/c: T32:=(H+u*c)*rho/(2)/c:
> T13:=1*rho/(2)/c: T23:=(u-c)*rho/(2)/c: T33:=(H-u*c)*rho/(2)/c:
> T:=array([ [T11, T12, T13], [T21, T22, T23], [T31, T32, T33]
]);
```

$$T := \begin{bmatrix} 1 & \frac{1}{2} \frac{\rho}{c} & \frac{1}{2} \frac{\rho}{c} \\ u & \frac{1}{2} \frac{(u+c)\rho}{c} & \frac{1}{2} \frac{(u-c)\rho}{c} \\ \frac{1}{2} u^2 & \frac{1}{2} \frac{(\frac{1}{2} u^2 + \frac{c^2}{\gamma-1} + cu)\rho}{c} & \frac{1}{2} \frac{(\frac{1}{2} u^2 + \frac{c^2}{\gamma-1} - cu)\rho}{c} \end{bmatrix}$$

```
> # (7) INVERSE OF EIGENVECTOR MATRIX:
> Tinv:=inverse(T);
```

$$T_{inv} := \begin{bmatrix} -\frac{1}{2} \frac{-u^2 + u^2 \gamma - 2c^2}{c^2} & \frac{u(\gamma-1)}{c^2} & -\frac{\gamma-1}{c^2} \\ \frac{1}{2} \frac{u(-u-2c+\gamma u)}{\rho c} & -\frac{-u-c+\gamma u}{\rho c} & \frac{\gamma-1}{\rho c} \\ \frac{1}{2} \frac{u(2c+\gamma u-u)}{\rho c} & -\frac{-u+c+\gamma u}{\rho c} & \frac{\gamma-1}{\rho c} \end{bmatrix}$$


```

> #
> # (8) DIAGONAL MATRIX OF EIGENVALUES:
> Lambda:=array([ [lambda[1], 0, 0], [0, lambda[2], 0], [0, 0,
lambda[3]] ]);

```

$$\Lambda := \begin{bmatrix} u & 0 & 0 \\ 0 & u + c & 0 \\ 0 & 0 & u - c \end{bmatrix}$$

```

> #
> # (9) QUESTION: VERIFY IF THE RELATION "T . LAMBDA . TINV" GIVES
> "A":

```

```

> AA:=multiply(T,Lambda,Tinv): AA:=simplify(%):
> DIFF:=matadd(A,-AA): DIFF:=simplify(%);

```

$$DIFF := \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

```

> #
> # (10) DIFFERENTIATE "Q" (NOTE dR = d Rho):
> deltaQ :=array([ [dR, u*dR+rho*du, dP/(gamma-1)+u^2/2*dR+rho*u*du]
]:
> deltaQ :=transpose(%);

```

$$\text{deltaQ} := \begin{bmatrix} dR \\ u dR + \rho du \\ \frac{dP}{\gamma - 1} + \frac{1}{2} u^2 dR + \rho u du \end{bmatrix}$$

```

> #
> # (11) DETERMINE WAVE AMPLITUDE BY MULTIPLYING "Tinv . deltaQ":
> dW:=multiply(Tinv, deltaQ): dW:=simplify(dW);

```

$$dW := \begin{bmatrix} \frac{dR c^2 - dP}{c^2} \\ \frac{c \rho du + dP}{\rho c} \\ -\frac{c \rho du - dP}{\rho c} \end{bmatrix}$$

Appendix C

Solution of the Fluid Equations by Upwind Differencing (UD) Schemes

C.1 Introduction

The numerical solution of the characteristic form, or decomposed form, of the fluid equations were obtained in Appendix B. That approach finds the Riemann invariants, w 's, in each new times step, then the w 's are related to the fluid primitive variables, to give ρ , p and u at each new time step. That approach is the direct solution of the decomposed form of the fluid equations. But as indicated in Appendix B, it is not the best possible solution of the multi-dimensional unsteady flows.

An alternative solution, which is still based on the numerical solution of the wave equation, is more appropriate and desired for computational fluid dynamics (CFD) applications. This approach can be more easily extended to multidimensional unsteady flows and will be addressed in this Appendix.

C.2 CFD Desired Numerical UD Schemes

Solutions of the characteristic form of the fluid equations are developed in Appendix B, as given by Eqns. B.39, B.40 and B.45, giving the Riemann invariants at the new time level. The Riemann invariants are therefore transformed to obtain density, pressure and velocity at the updated time step. Eqns. B.39, B.40 and B.45 could be written in a compact form in the following vector equations:

$$W_j^{n+1} = W_j^n - \frac{\Delta t}{\Delta x} \left[[\Lambda^+] (W_j^n - W_{j-1}^n) + [\Lambda^-] (W_{j+1}^n - W_j^n) \right], \quad (C.1)$$

or

$$W_j^{n+1} = W_j^n - \frac{\Delta t}{2\Delta x} [\Lambda] [W_{j+1}^n - W_{j-1}^n] + \frac{\Delta t}{2\Delta x} [|\Lambda|] [W_{j+1}^n - 2W_j^n + W_{j-1}^n] \quad (C.2)$$

Eqn. C.1 is consistent with that type of solution of the wave equation given by Eqn. A.19 (FVS form of the wave equation) and Eqn. C.2 is consistent with Eqn. A.23 (FDS form of the wave equation). It is noted that in Eqns. C.1 and C.2, W is the Riemann invariants vector, which satisfies Eqn. B.24, $[\Lambda^+]$ is a diagonal matrix with its elements being the positive (or zero) eigenvalues, i.e. λ^+ 's (or 0) and, $[\Lambda^-]$ is a diagonal matrix with its elements being the negative eigenvalues, i.e. λ^- 's. The following equation could also be used to obtain $[\Lambda^-]$:

$$[\Lambda^-] = [\Lambda] - [\Lambda^+]. \quad (C.3)$$

As mentioned earlier, the solution of the decomposed form of the fluid equations are not totally suitable for fluid equations, therefore another alternative, which is more suitable for the computational fluid dynamics (CFD) applications is sought. In this approach, similar to the method of solution for the characteristic form of the fluid equations as outlined in section B.3.2, Eqn. C.1 is used. However before obtaining the Riemann invariants at the new time step, Eqn. C.1 is transformed from the domain of Riemann invariants to the domain of primitive variables. This transformation is performed by:

$$\delta Q = [T] \delta W \quad (C.4)$$

In fact, Eqn. C.4 is in the opposite direction of Eqn. B.23 (it should be recalled that Eqn. B.23 was used to transform the fluid equations into the characteristic form, and now Eqn. C.4 is applied to transform back the solution from the characteristic domain into the original domain of primitive variables). This transforming back to the domain of primitive variables bypasses an intermediate step, in which updated values of Riemann invariants are calculated. Therefore, some computational costs are saved. Moreover the resulting equations are more suitable for the CFD applications and can be easily extended to multi-dimensional unsteady flows. Also in this approach the physical flow variables like pressure, density and velocity components are dealt with rather than un-physically measurable parameters of the Riemann invariants.

Two different algorithms were applied to the wave equation in Appendix A, namely FVS and FDS, in which the basic equations of FVS and FDS were obtained (Eqns. A.19 for FVS and A.23 for FDS). The same principles are generalized here as the method is extended to fluid equations. Eqn. C.1 will be used for FVS and Eqn. C.2 for the FDS.

C.3 Development of the FVS Scheme as Applied to Fluid Equations

Discretization of fluid equations by the FVS scheme is developed in this section. Eqn. C.1 is very similar in form to Eqn. A.19 (recall that Eqn. A.19 is the discretized form of the wave equation by the FVS scheme). Eqn. C.1 is transformed to the domain of primitive variables as follows.

Multiplying Eqn. C.1 by gives:

$$[T]W_j^{n+1} = [T]W_j^n - \frac{\Delta t}{\Delta x} \left[[T][\Lambda^+] (W_j^n - W_{j-1}^n) + [T][\Lambda^-] (W_{j+1}^n - w_{2j}^n) \right] \quad (C.5)$$

Using Eqn. C.4, it can be shown that:

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x} \left[[T][\Lambda^+] (W_j^n - W_{j-1}^n) + [T][\Lambda^-] (W_{j+1}^n - w_{2j}^n) \right] \quad (C.6)$$

and substituting $\delta W = [T]^{-1} \delta Q$ according to Eqn. B.23 gives:

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x} \left[[T][\Lambda^+][T]^{-1} (Q_j^n - Q_{j-1}^n) + [T][\Lambda^-][T]^{-1} (Q_{j+1}^n - Q_j^n) \right]. \quad (\text{C.7})$$

On the other hand according to Eqn. B.16:

$$[A^+] = [T][\Lambda^+][T]^{-1}, \quad (\text{C.8})$$

$$[A^-] = [T][\Lambda^-][T]^{-1}. \quad (\text{C.9})$$

It is noted that $[A^-]$ could also be determined from:

$$[A^-] = [A] - [A^+]. \quad (\text{C.10})$$

Finally, the discretized form of the fluid equation by the FVS scheme is obtained:

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x} \left[[A^+] (Q_j^n - Q_{j-1}^n) + [A^-] (Q_{j+1}^n - Q_j^n) \right]. \quad (\text{C.11})$$

As shown in section B.2.1, F is a homogenous function of components Q , therefore, according to Eqn. B.9 one can write:

$$F^+ = [A^+]Q, \quad (\text{C.12})$$

$$F^- = [A^-]Q. \quad (\text{C.13})$$

Therefore, another form for the discretized fluid equations could be obtained as:

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x} \left[(F_j^{+n} - F_{j-1}^{+n}) + (F_{j+1}^{-n} - F_j^{-n}) \right]. \quad (\text{C.14})$$

Eqn. C.14 could also be written in the following form:

$$Q_j^{n+1} = Q_j^n - \Delta t \left[\left(\frac{F_j^{+n} - F_{j-1}^{+n}}{\Delta x} \right) + \left(\frac{F_{j+1}^{-n} - F_j^{-n}}{\Delta x} \right) \right]. \quad (\text{C.15})$$

Either of the Eqns. C.11, C.14 or C.15 is the discretized form of the governing equation of fluid motion by FVS schemes. Consider Eqn. C.15 for example, it implies backward difference for F^+ and forward difference for F^- , which totally agrees with the essence of upwinding (it is recalled that F^+ corresponds to positive eigenvalues-information coming from upstream and F^- corresponds to negative eigenvalues-information coming from downstream). Summary of FVS for fluid equations is given below.

C.3.1 Summary of FVS Formulation for Fluid Equations

The following steps are taken to discretize the fluid equations by an FVS scheme:

1. Determine the eigenvalues of the Jacobian matrix from Eqn. B.13.
2. According to the sign of the eigenvalues, obtain $[\Lambda^+]$. Then:

$$[\Lambda^-] = [\Lambda] - [\Lambda^+] \quad (\text{C.16})$$

3. Determine $[A^+]$ from Eqn. C.8. Then:

$$[A^-] = [A] - [A^+]. \quad (\text{C.17})$$

4. Obtain F^+ from Eqn. C.12. Then:

$$F^- = F - F^+. \quad (\text{C.18})$$

5. Split the flux vector F into positive and negative terms ($F = F^+ + F^-$), then find its space derivative:

$$\frac{\partial F}{\partial x} = \frac{\partial}{\partial x}(F^+ + F^-). \quad (\text{C.19})$$

6. Determine each element of Eqn. C.19 by using backward difference in space for F^+ terms and forward difference for F^- :

$$\frac{\partial F^+}{\partial x} = \frac{F_j^{+n} - F_{j-1}^{+n}}{\Delta x}, \quad \frac{\partial F^-}{\partial x} = \frac{F_{j+1}^{-n} - F_j^{-n}}{\Delta x} \quad (\text{C.20})$$

7. For the time discretization apply, say, first order forward difference:

$$\frac{\partial Q}{\partial t} = \frac{Q_j^{n+1} - Q_j^n}{\Delta t}. \quad (\text{C.21})$$

8. Therefore, the numerical solution for the Euler equation given by Eqn. 2.5 becomes.

$$Q_j^{n+1} = Q_j^n - \Delta t \left[\left(\frac{F_j^{+n} - F_{j-1}^{+n}}{\Delta x} \right) + \left(\frac{F_{j+1}^{-n} - F_j^{-n}}{\Delta x} \right) \right]. \quad (\text{C.22})$$

It is noted that this is equivalent to Eqn. C.15.

C.4 Development of Flux Difference Splitting (FDS) Scheme as Applied to Fluid Equations

Eqn. C.1 was used to discretize the fluid equations by an FVS scheme. In this section Eqn. C.2 will be used to develop the discretized equations of fluid motion by an FDS scheme.

As with the FVS algorithm, in which Eqn. C.1 was transformed into the primitive variables domain, Eqn. C.2 is transformed to the primitive variables domain. Multiplying $[T]$ by Eqn. C.2:

$$[T]W_j^{n+1} = [T]W_j^n - \frac{\Delta t}{2\Delta x} [T][\Lambda][W_{j+1}^n - W_{j-1}^n] + \frac{\Delta t}{2\Delta x} [T][|\Lambda|][W_{j+1}^n - 2W_j^n + W_{j-1}^n] \quad (C.23)$$

Using Eqn. C.4, one can write:

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{2\Delta x} [T][\Lambda][W_{j+1}^n - W_{j-1}^n] + \frac{\Delta t}{2\Delta x} [T][|\Lambda|][W_{j+1}^n - 2W_j^n + W_{j-1}^n] \quad (C.24)$$

Also substituting $\delta W = [T]^{-1} \delta Q$ according to Eqn. B.23:

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{2\Delta x} [T][\Lambda][T]^{-1} [Q_{j+1}^n - Q_{j-1}^n] + \frac{\Delta t}{2\Delta x} [T][|\Lambda|][T]^{-1} [Q_{j+1}^n - 2Q_j^n + Q_{j-1}^n] \quad (C.25)$$

and recalling from Eqn. B.16 that $[A] = [T][\Lambda][T]^{-1}$, also defining $[|A|]$ as:

$$[|A|] \equiv [T][|\Lambda|][T]^{-1} \quad (C.26)$$

Therefore, Eqn. C.25 could be written as:

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{2\Delta x} [A] [Q_{j+1}^n - Q_{j-1}^n] + \frac{\Delta t}{2\Delta x} [|A|] [Q_{j+1}^n - 2Q_j^n + Q_{j-1}^n] \quad (C.27)$$

On the other hand, $F = [A]Q$ according to the fact that F is a homogenous function of the components of Q (see Eqn. B.9). Therefore:

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{2\Delta x} [F_{j+1}^n - F_{j-1}^n] + \frac{\Delta t}{2\Delta x} [|A|] [Q_{j+1}^n - 2Q_j^n + Q_{j-1}^n]. \quad (C.28)$$

Eqn. C.28 is very similar to Eqn. A.23 (recall that Eqn. A.23 is the discretized form of the wave equation by the FDS scheme). Similar to Eqn. A.26, the numerical fluxes

for the fluid equation can also be represented in the same way that the numerical fluxes of the wave equations were obtained:

$$f_E = \frac{1}{2} [F_j^n + F_{j+1}^n] - \frac{1}{2} [|A|] (Q_{j+1}^n - Q_j^n) \quad (\text{C.29})$$

and

$$f_W = \frac{1}{2} [F_j^n + F_{j-1}^n] - \frac{1}{2} [|A|] (Q_j^n - Q_{j-1}^n) \quad (\text{C.30})$$

where f_E and f_W are shown in Fig.C.1. Finally, the numerical solution of the Euler equation, Eqn. 2.5, could be given by:

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x} (f_E - f_W). \quad (\text{C.31})$$

It is noted that Eqn. C.31 with the numerical fluxes f_E and f_W given by Eqns. C.29 and C.30 define the discretized form for the Euler equation, which is equivalent to Eqn. C.28.

The numerical fluxes represented by Eqns. C.29 and C.30 imply the basics of one of the most popular FDS algorithms introduced by Roe (1981). However, Roe computes $[|A|]$ in a so called Roe's averaged condition and it is denoted by $[|\hat{A}|]$ in his numerical flux formulation. It is noted that $[|\hat{A}|]$ has the same form as $[|A|]$, as given by Eqn. B.7, unless it is evaluated at Roe's averaged condition. This averaging is performed at each cell-face, and is determined from left- and right- contribution of the primitive variables at each cell-face. For the current study, the Roe scheme will be totally applied for in the space discretization. Therefore, the formulation of the Roe scheme as applied to fluid equations deserves to be brought in a separate Appendix (Appendix D).

C.5 Conclusion

The numerical solution of the fluid equation by upwind differencing (UD) schemes are developed based on the numerical solution of the wave equation (or the characteristic form of the fluid equation). This solution is in fact developed based on the physics of traveling waves (or disturbances), in which it takes into account the side from which information arrives at the point of interest. This has been the main

Figure C.1: Numerical fluxes of f_E and f_W corresponding to the node j .

motivation for bypassing an easy and symmetric discretization method, i.e., central differencing (CD) algorithms, which are blind in detecting the side from which the information arrives at the point of interest.

In the current Appendix the basics of the two major categories of upwind differencing schemes are explained, namely the flux vector splitting (FVS) scheme and the flux differencing splitting (FDS) scheme.

Discussing of the advantages and disadvantages of these schemes may be found in Chapter 2. Appendices B, C and D are only intended to include the formulations for these schemes and keep the formulae development away from the main context (and contributions) of this thesis. However, it is worthwhile to mention here that the most important FVS schemes are those which have been developed by Steger and Warming (1981) and Van-Leer (1982) and the most popular FDS scheme is that due to Roe (1981). No more material about FVS schemes are given in these appendices. However for the FDS scheme of Roe (1981), as it will be applied throughout the course of this thesis, an Appendix, Appendix D, is totally devoted to the development of the Roe scheme as applied to fluid equations.

Appendix D

Roe's FDS Scheme for Fluid Equations

D.1 Introduction

As indicated in section 4.1, Exact Riemann Solver (ERS) schemes are not computationally efficient for the iterative solution of the fluid equations. However, one idea that has been used with good success in computing the solution of fluid equation (which are a set of non-linear coupled equations) is to use Approximate Riemann Solvers (ARS) rather than ERS. Roe's method (1981) is one of the most popular ARS schemes. Roe's linear approximation to the Riemann problem suggests that to solve the linear problem; written as:

$$\frac{\partial Q}{\partial t} + [\hat{A}] \frac{\partial Q}{\partial x} = 0 \quad (\text{D.1})$$

where $[\hat{A}]$ is the Jacobian matrix estimated at Roe's averaged condition. This matrix appears as locally constant in each iteration at the time frame of reference. $[\hat{A}]$ is constructed to satisfy certain conditions, the so called U conditions by Roe.

In this Appendix, the application of Roe's scheme to one dimensional flow is explained first. This is followed by extending the method to two dimensional unsteady flows. Later on it will be extended to multidimensional cases.

Consider the distribution of a series of nodes along a string as shown in Fig D.1. Numerical flux at the East side (E) of an arbitrary cell is calculated and is denoted

Figure D.1: Distribution of a series of nodes along a string. Each node is confined with its East (E) and West (W) cell faces, where only face E is shown here. Two values, namely, Left (L) and Right (R) are specified at each cell face, and numerical flux f_E is determined based on the L and R values. jjj is the number of nodes along the string.

by f_{E_j} as shown for node $j = 2$ in Fig D.1 for example. This could be extended to all nodes providing the magnitude of numerical flux at the East face of all cells. Once f_{E_j} for all the nodes are determined, the numerical flux at the West (W) face of a cell, f_{W_j} is $f_{E_{j-1}}$. Then it is said that the space discretization is concluded. The time discretization, therefore, must be obtained. For the time discretization (like space discretization) any degree of accuracy could be sought. In this Appendix, first order accurate scheme for both the time and space are given as:

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x} (f_{E_j} - f_{W_j}) \quad (\text{D.2})$$

Higher order of accuracy of the scheme, the so called *high resolution schemes*, are explained in sections 6.4 and 6.5 and in Kermani and Plett (2001^c).

D.2 Roe Scheme for 1-D Fluid Equations; Summary of Formulae

The space discretization procedure of the first order Roe scheme is given in this section. Higher order space discretization are given in sections 6.4 and 6.5. The space discretization of fluid equations by Roe scheme (1981) could be given in different ways. The following approach is popularly reported in the literature, see Hirsch (1990) for example, and is given here.

1. Primitive variables at the left and right sides of each cell face are approximated by:

$$\begin{aligned}\rho_E^L &= \rho_j & \rho_E^R &= \rho_{j+1} \\ u_E^L &= u_j & u_E^R &= u_{j+1} \\ H_E^L &= H_j & H_E^R &= H_{j+1}\end{aligned}\tag{D.3}$$

where H is the total specific enthalpy, $H = \frac{\gamma}{\gamma-1} \frac{p}{\rho} + \frac{u^2}{2}$. It is noted that this is first order approximation for the estimation of fluid primitive variables. For the current study a third order upwind biased scheme for the space discretization is utilized using the MUSCL idea as introduced by van Leer (1979) and explained in section 6.5.

2. the square root of density at the Left (L) and Right (R) sides of E are obtained and are taken as the weighting factors. These determine the contribution from each side of the cell:

$$W_E^L = \sqrt{\rho_E^L}, \quad W_E^R = \sqrt{\rho_E^R}.\tag{D.4}$$

3. Primitive variables at the cell face E are determined by W_E^L and W_E^R contributions from L and R values of primitive variables. These determine the, so-called *Roe averaged condition* and are denoted by hat, $\hat{\cdot}$,

$$\hat{\rho}_E \equiv W_E^L \rho_E^L + W_E^R \rho_E^R\tag{D.5}$$

$$\hat{u}_E \equiv \frac{W_E^L u_E^L + W_E^R u_E^R}{W_E^L + W_E^R}\tag{D.6}$$

$$\hat{H}_E \equiv \frac{W_E^L H_E^L + W_E^R H_E^R}{W_E^L + W_E^R}.\tag{D.7}$$

4. Speed of sound at the Roe averaged condition is determined as:

$$\hat{c}_E = \sqrt{(\gamma - 1) \left(\hat{H}_E - \frac{\hat{u}_E^2}{2} \right)}.\tag{D.8}$$

5. Eigenvalues of the Jacobian matrix are, therefore, determined from Eqn. B.13 at the Roe averaged condition:

$$\hat{\lambda}_E^{(1)} = \hat{u}_E, \quad \hat{\lambda}_E^{(2)} = \hat{u}_E + \hat{c}_E, \quad \hat{\lambda}_E^{(3)} = \hat{u}_E - \hat{c}_E. \quad (\text{D.9})$$

6. The corresponding eigenvectors are also determined from Eqn. B.15 at Roe averaged condition:

$$\hat{T}_E^{(1)} = \begin{bmatrix} 1 \\ \hat{u}_E \\ \frac{\hat{u}_E^2}{2} \end{bmatrix}, \quad \hat{T}_E^{(2)} = \begin{bmatrix} 1 \\ \hat{u}_E + \hat{c}_E \\ \hat{H}_E + \hat{u}_E \hat{c}_E \end{bmatrix} \frac{\hat{\rho}_E}{2\hat{c}_E}, \quad \hat{T}_E^{(3)} = \begin{bmatrix} 1 \\ \hat{u}_E - \hat{c}_E \\ \hat{H}_E - \hat{u}_E \hat{c}_E \end{bmatrix} \frac{\hat{\rho}_E}{2\hat{c}_E}. \quad (\text{D.10})$$

7. The increment of the primitive variables p , ρ , and u at the cell face E are, therefore, determined:

$$\delta p_E = p_E^R - p_E^L, \quad \delta \rho_E = \rho_E^R - \rho_E^L, \quad \delta u_E = u_E^R - u_E^L. \quad (\text{D.11})$$

8. Therefore, the wave amplitude vector is obtained according to the Eqn. B.24:

$$\delta W_E \equiv \begin{bmatrix} \delta w_E^{(1)} \\ \delta w_E^{(2)} \\ \delta w_E^{(3)} \end{bmatrix} = \begin{bmatrix} \delta \rho_E - \frac{\delta p_E}{\hat{c}_E} \\ \delta u_E + \frac{\delta p_E}{\hat{\rho}_E \hat{c}_E} \\ -\delta u_E + \frac{\delta p_E}{\hat{\rho}_E \hat{c}_E} \end{bmatrix}. \quad (\text{D.12})$$

9. Finally the numerical flux at the cell face E is determined according to Eqn. C.29:

$$f_E = \frac{1}{2} (F_E^L + F_E^R) - \frac{1}{2} \sum_{\kappa=1}^3 |\hat{\lambda}_E^{(\kappa)}| \delta w_E^{(\kappa)} \hat{T}_E^{(\kappa)} \quad (\text{D.13})$$

where each κ corresponds to each wave propagating in the $x - t$ domain. Eqn. D.13 could be simplified by expanding the summation as:

$$f_E = \frac{1}{2} (F_E^L + F_E^R) - \frac{1}{2} [\Delta F_E^{(1)} + \Delta F_E^{(2)} + \Delta F_E^{(3)}]. \quad (\text{D.14})$$

It is noted that all the elements of Eqn. D.14 are a three element vector for the one-dimensional computation, and they are defined as follows:

Figure D.2: Flux values at Left (L) and Right (R) of the East (E) cell face.

The vector f_E in the L.H.S of Eqn. D.14 is:

$$f_E \equiv \begin{bmatrix} (f_E)_{Cont.} \\ (f_E)_{Mom.} \\ (f_E)_{Engy.} \end{bmatrix}, \quad (D.15)$$

On the R.H.S., F_E^L and F_E^R are obtained by a first order accurate scheme (see Fig. D.2):

$$F_E^L = F_j = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (\rho e_t + p)u \end{bmatrix}_j, \quad F_E^R = F_{j+1} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (\rho e_t + p)u \end{bmatrix}_{j+1}, \quad (D.16)$$

and

$$\Delta F_E^{(1)} \equiv |\hat{\lambda}_E^{(1)}| \delta w_E^{(1)} \hat{T}_E^{(1)} \quad (D.17)$$

$$\Delta F_E^{(2)} \equiv |\hat{\lambda}_E^{(2)}| \delta w_E^{(2)} \hat{T}_E^{(2)} \quad (D.18)$$

$$\Delta F_E^{(3)} \equiv |\hat{\lambda}_E^{(3)}| \delta w_E^{(3)} \hat{T}_E^{(3)} \quad (D.19)$$

or ΔF_E 's in expanded form:

$$\Delta F_E^{(1)} = |\hat{u}_E| \left(\delta \rho_E - \frac{\delta p_E}{\hat{c}_E^2} \right) \begin{bmatrix} 1 \\ \hat{u}_E \\ \frac{\hat{u}_E^2}{2} \end{bmatrix} \quad (D.20)$$

$$\Delta F_E^{(2)} = |\hat{u}_E + \hat{c}_E| \left(\frac{\delta p_E}{\hat{\rho}_E \hat{c}_E} + \delta u_E \right) \begin{bmatrix} 1 \\ \hat{u}_E + \hat{c}_E \\ \hat{H}_E + \hat{u}_E \hat{c}_E \end{bmatrix} \frac{\hat{\rho}_E}{2\hat{c}_E} \quad (D.21)$$

$$\Delta F_E^{(3)} = |\hat{u}_E - \hat{c}_E| \left(\frac{\delta p_E}{\hat{\rho}_E \hat{c}_E} - \delta u_E \right) \begin{bmatrix} 1 \\ \hat{u}_E - \hat{c}_E \\ \hat{H}_E - \hat{u}_E \hat{c}_E \end{bmatrix} \frac{\hat{\rho}_E}{2\hat{c}_E}. \quad (\text{D.22})$$

The one dimensional formulation of the Roe scheme has been explained in this section. One dimensional approximations of flow simulations are limited to a very few simple applications like the shock tube problem. The shock tube problem, although it is a simple problem, contains all the challenging elements of fluid flow which is very suitable to evaluate the predictability of the numerical schemes. These elements in particular are: shock waves, contact discontinuities, and expansion waves in unsteady frame of reference. The shock tube problem is studied by the current approach and the results are benchmarked against analytical results (see chapter 4 or Kermani and Plett (2001^a)).

The discretization of one-dimensional fluid equations by the Roe scheme has successfully been completed. Two-dimensional discretization of fluid equations by the Roe scheme in generalized coordinates are given in chapter 5 of this thesis and in Kermani and Plett (2001^b).

D.3 Riemann Problem

The shock tube problem is often referred to as the *Riemann problem* in the literature. The Riemann problem is addressed here.

D.4 Roe Scheme for 2-D Fluid Equations; over Arbitrary Grid

The governing equations of fluid motion in two-dimensional inviscid flow with no body force and in full conservative form is:

$$\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0 \quad (\text{D.23})$$

where the conservative vector Q and the flux vectors F and G are:

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho e_t \end{bmatrix}, \quad F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho u H \end{bmatrix}, \quad G = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho v H \end{bmatrix}, \quad (\text{D.24})$$

where e_t is the total specific internal energy ($e_t = e + \frac{1}{2}V^2$), $V^2 = u^2 + v^2$ and $H = h + \frac{1}{2}V^2$.

D.4.1 Roe Scheme for 2-D Fluid Equations; Summary of Formulae

The grid configuration assumed here, could be any type and the control volume associated with a node considers the boundary of the control volume to be at the mid-point between two adjacent nodes. The numerical flux crossing one face of this control volume, say face l , by a first order accurate scheme in space is obtained in this section (for higher order of accuracy, the reader is referred to sections 6.4 and 6.5). It is noted for any face of a given control volume that the superscript L corresponds to the inner value and R corresponds to outer value.

Fig. D.3 shows node (j, k) with the neighboring nodes surrounding this node, namely $(j+1, k)$, $(j-1, k)$, $(j, k+1)$, and $(j, k-1)$. Also the corresponding control volumes associated with all of these nodes are sketched there. The goal of this section is to obtain the numerical flux at an arbitrary face of the control volume corresponding to the node (j, k) , say face l .

1. Primitive variables at the L and R sides of the cell face l (if l corresponds to the face AB) are approximated by: (it is noted that this is a first order approximation for the extrapolation of fluid properties)

$$\begin{aligned} \rho_l^L &= \rho_{j,k} & \rho_l^R &= \rho_{j+1,k} \\ u_l^L &= u_{j,k} & u_l^R &= u_{j+1,k} \end{aligned} \quad (\text{D.25})$$

$$v_l^L = v_{j,k} \quad v_l^R = v_{j+1,k} \quad (\text{D.26})$$

$$H_l^L = H_{j,k} \quad H_l^R = H_{j+1,k}$$

Figure D.3: Arbitrary configuration of grid lines with the corresponding cell-vertex control volume allocated to each node. Grid lines are shown by solid lines and control volume boundaries with dashed-lines.

where H is the total specific enthalpy, given by $H = \frac{\gamma}{\gamma-1} \frac{p}{\rho} + \frac{u^2+v^2}{2}$.

If l corresponds to the face BC then:

$$\begin{aligned} \rho_l^L &= \rho_{j,k} & \rho_l^R &= \rho_{j,k+1} \\ u_l^L &= u_{j,k} & u_l^R &= u_{j,k+1} \end{aligned} \quad (D.27)$$

$$\begin{aligned} v_l^L &= v_{j,k} & v_l^R &= v_{j,k+1} \end{aligned} \quad (D.28)$$

$$\begin{aligned} H_l^L &= H_{j,k} & H_l^R &= H_{j,k+1} \end{aligned}$$

Once the u and v components of velocity are determined at the cell face l then $u_{\perp}$ and $u_{\parallel}$ are obtained as follows:

$$u_{\perp}^L = u_l^L \cos\theta_l + v_l^L \sin\theta_l, \quad u_{\parallel}^L = -u_l^L \sin\theta_l + v_l^L \cos\theta_l, \quad (D.29)$$

$$u_{\perp}^R = u_l^R \cos\theta_l + v_l^R \sin\theta_l, \quad u_{\parallel}^R = -u_l^R \sin\theta_l + v_l^R \cos\theta_l, \quad (D.30)$$

Figure D.4: Arbitrary shaped control volume in two-dimensional flow.

where θ_l is the angle of the cell face vector subtended with the x axis, see Fig. D.4.

2. The square root of density at the L and R side of the cell face l are determined in order to apply them as the weighting factors:

$$W_l^L = \sqrt{\rho_l^L}, \quad W_l^R = \sqrt{\rho_l^R}. \quad (\text{D.31})$$

3. Roe's averaged primitive variables at the cell face l are determined by appropriate contribution from L and R sides of the face:

$$\hat{\rho}_l \equiv W_l^L W_l^R \quad (\text{D.32})$$

$$\hat{u}_l \equiv \frac{W_l^L u_l^L + W_l^R u_l^R}{W_l^L + W_l^R} \quad (\text{D.33})$$

$$\hat{v}_l \equiv \frac{W_l^L v_l^L + W_l^R v_l^R}{W_l^L + W_l^R} \quad (\text{D.34})$$

$$\hat{H}_l \equiv \frac{W_l^L H_l^L + W_l^R H_l^R}{W_l^L + W_l^R}. \quad (\text{D.35})$$

Therefore,

$$\hat{u}_{\perp l} = \hat{u}_l \cos\theta_l + \hat{v}_l \sin\theta_l, \quad \hat{u}_{\parallel l} = -\hat{u}_l \sin\theta_l + \hat{v}_l \cos\theta_l. \quad (\text{D.36})$$

4. Speed of sound is determined as follows:

$$\hat{c}_l = \sqrt{(\gamma - 1) \left(\hat{H}_l - \frac{\hat{u}_l^2 + \hat{v}_l^2}{2} \right)}. \quad (\text{D.37})$$

5. Eigenvalues at the cell face l are:

$$\begin{bmatrix} \hat{\lambda}_l^{(1)} \\ \hat{\lambda}_l^{(2)} \\ \hat{\lambda}_l^{(3)} \\ \hat{\lambda}_l^{(4)} \end{bmatrix} = \begin{bmatrix} \hat{u}_{\perp l} - \hat{c}_l \\ \hat{u}_{\perp l} \\ \hat{u}_{\perp l} \\ \hat{u}_{\perp l} + \hat{c}_l \end{bmatrix}. \quad (\text{D.38})$$

6. The corresponding eigenvectors at the cell face l are:

$$\begin{aligned} \hat{T}_l^{(1)} &= \begin{bmatrix} 1 \\ \hat{u}_l - \hat{c}_l \cos\theta_l \\ \hat{v}_l - \hat{c}_l \sin\theta_l \\ \hat{H}_l - \hat{u}_{\perp l} \hat{c}_l \end{bmatrix}, \quad \hat{T}_2^{(2)} = \begin{bmatrix} 0 \\ -\sin\theta_l \\ \cos\theta_l \\ \hat{u}_{\parallel l} \end{bmatrix}, \quad \hat{T}_3^{(3)} = \begin{bmatrix} 1 \\ \hat{u}_l \\ \hat{v}_l \\ \frac{\hat{u}_l^2 + \hat{v}_l^2}{2} \end{bmatrix}, \\ \hat{T}_4^{(4)} &= \begin{bmatrix} 1 \\ \hat{u}_l + \hat{c}_l \cos\theta_l \\ \hat{v}_l + \hat{c}_l \sin\theta_l \\ \hat{H}_l + \hat{u}_{\perp l} \hat{c}_l \end{bmatrix}. \end{aligned} \quad (\text{D.39})$$

7. The increment of the primitive variables at the cell face l are:

$$\delta p_l = p_l^R - p_l^L, \quad \delta \rho_l = \rho_l^R - \rho_l^L, \quad \delta u_{\perp l} = u_{\perp l}^R - u_{\perp l}^L, \quad \delta u_{\parallel l} = u_{\parallel l}^R - u_{\parallel l}^L. \quad (\text{D.40})$$

8. The wave amplitude vector is obtained as follows:

$$\delta W_l \equiv \begin{bmatrix} \delta w_l^{(1)} \\ \delta w_l^{(2)} \\ \delta w_l^{(3)} \\ \delta w_l^{(4)} \end{bmatrix} = \begin{bmatrix} \frac{\delta p_l - \hat{\rho}_l \hat{c}_l \delta u_{\perp l}}{2 \hat{c}_l^2} \\ \hat{\rho}_l \delta u_{\parallel l} \\ - \frac{\delta p_l - \hat{c}_l^2 \delta \rho_l}{\hat{c}_l^2} \\ \frac{\delta p_l + \hat{\rho}_l \hat{c}_l \delta u_{\perp l}}{2 \hat{c}_l^2} \end{bmatrix}. \quad (\text{D.41})$$

9. Finally the numerical flux R_{l_n} is:

$$R_{l_n} = \frac{1}{2} [R_{l_n}^L + R_{l_n}^R] - \frac{1}{2} [\Delta R_l^{(1)} + \Delta R_l^{(2)} + \Delta R_l^{(3)} + \Delta R_l^{(4)}] \quad (\text{D.42})$$

where all the elements of the Eqn. D.42 are a four element vector for the two-dimensional computation; the inner (L) and outer (R) flux components in the normal direction of the cell face l are:

$$R_{l_n}^L = \begin{bmatrix} \rho u_{\perp} \\ \rho u u_{\perp} + p \cos \theta \\ \rho v u_{\perp} + p \sin \theta \\ \rho u_{\perp} H \end{bmatrix}_l^L, \quad R_{l_n}^R = \begin{bmatrix} \rho u_{\perp} \\ \rho u u_{\perp} + p \cos \theta \\ \rho v u_{\perp} + p \sin \theta \\ \rho u_{\perp} H \end{bmatrix}_l^R; \quad (\text{D.43})$$

and the diffusion terms corresponding to each wave are:

$$\Delta R_l^{(1)} \equiv |\hat{\lambda}_l^{(1)}| \delta w_l^{(1)} \hat{T}_l^{(1)} \quad (\text{D.44})$$

$$\Delta R_l^{(2)} \equiv |\hat{\lambda}_l^{(2)}| \delta w_l^{(2)} \hat{T}_l^{(2)} \quad (\text{D.45})$$

$$\Delta R_l^{(3)} \equiv |\hat{\lambda}_l^{(3)}| \delta w_l^{(3)} \hat{T}_l^{(3)} \quad (\text{D.46})$$

$$\Delta R_l^{(4)} \equiv |\hat{\lambda}_l^{(4)}| \delta w_l^{(4)} \hat{T}_l^{(4)} \quad (\text{D.47})$$

or ΔR_l 's in expanded form:

$$\Delta R_l^{(1)} = |\hat{u}_{\perp l} - \hat{c}_l| \left(\frac{\delta p_l - \hat{\rho}_l \hat{c}_l \delta u_{\perp l}}{2 \hat{c}_l^2} \right) \begin{bmatrix} 1 \\ \hat{u}_l - \hat{c}_l \cos \theta_l \\ \hat{v}_l - \hat{c}_l \sin \theta_l \\ \hat{H}_l - \hat{u}_{\perp l} \hat{c}_l \end{bmatrix}, \quad (\text{D.48})$$

$$\Delta R_l^{(2)} = |\hat{u}_{\perp l}| \left(\hat{\rho}_l \delta u_{\parallel l} \right) \begin{bmatrix} 0 \\ -\sin\theta_l \\ \cos\theta_l \\ \hat{u}_{\parallel l} \end{bmatrix}, \quad (\text{D.49})$$

$$\Delta R_l^{(3)} = |\hat{u}_{\perp l}| \left(-\frac{\delta p_l - \hat{c}_l^2 \delta \rho_l}{\hat{c}_l^2} \right) \begin{bmatrix} 1 \\ \hat{u}_l \\ \hat{v}_l \\ \frac{\hat{u}_l^2 + \hat{v}_l^2}{2} \end{bmatrix}, \quad (\text{D.50})$$

$$\Delta R_l^{(4)} = |\hat{u}_{\perp l} + \hat{c}_l| \left(\frac{\delta p_l + \hat{\rho}_l \hat{c}_l \delta u_{\perp l}}{2 \hat{c}_l^2} \right) \begin{bmatrix} 1 \\ \hat{u}_l + \hat{c}_l \cos\theta_l \\ \hat{v}_l + \hat{c}_l \sin\theta_l \\ \hat{H}_l + \hat{u}_{\perp l} \hat{c}_l \end{bmatrix}. \quad (\text{D.51})$$

The discretization of the two-dimensional fluid equations by the Roe scheme is concluded here as the numerical flux crossing a cell face of an arbitrarily shaped control volume is obtained.

D.5 Conclusion

The formulation of the Roe scheme for one-dimensional and two-dimensional fluid equations are given in this Appendix. The discretization of the Roe scheme in generalized coordinates is given in chapter 5 and in Kermani and Plett (2001^b).

Appendix E

Publications Relating to this Thesis

1. Kermani, M. J. and Plett, E. G., Laminar Supersonic Flow Between Parallel Plates; Analysis by MacCormack Scheme, Fourth Annual Conference of the CFD Society of Canada, Ottawa, Ontario, Canada, June 2-6, 1996.
2. Kermani, M. J. and Plett, E. G., Development of a Second Order Upwind Scheme with Application to Supersonic Euler Flow, AIAA 1998-0930, 1998, Presented at the 36th Aerospace Science Meeting and Exhibit, Reno, Nevada.
3. Kermani, M. J. and Plett, E. G., Application of a Combined Second- and Third-Order Scheme into Axisymmetric Supersonic Euler Flow, Sixth Annual Conference of the CFD Society of Canada, Quebec City, Canada, June 7-9, 1998.
4. Kermani, M. J. and Plett, E. G. Modified Entropy Correction Formula for the Roe Scheme, AIAA 2001-0083, 2001, Presented at the 39th Aerospace Science Meeting and Exhibit, Reno, Nevada.
5. Kermani, M. J. and Plett, E. G. Roe Scheme in Generalized Coordinates; Part I- Formulations, AIAA 2001-0086, 2001, Presented at the 39th Aerospace Science Meeting and Exhibit, Reno, Nevada.

6. Kermani, M. J. and Plett, E. G. Roe Scheme in Generalized Coordinates;
Part II- Application to Inviscid and Viscous Flows, AIAA 2001-0087, 2001,
Presented at the 39th Aerospace Science Meeting and Exhibit, Reno, Nevada.