NUMERICAL SIMULATION OF HYPersonic
Laminar FLOW OVER A BLUNT CONE FLARE

By

CHUWEI CHEN

A dissertation submitted to the
School of Graduate Studies
Rutgers, The State University of New Jersey
In partial fulfillment of the requirements
For the degree of
Doctor of Philosophy
Graduate Program in Mechanical and Aerospace Engineering

Written under the direction of
Doyle D. Knight
and approved by

__________________________
__________________________
__________________________
__________________________

New Brunswick, New Jersey
January, 2022
ABSTRACT OF THE DISSERTATION

Numerical Simulation of Hypersonic Laminar Flow Over a Blunt Cone Flare

by Chuwei Chen

Dissertation Director:

Doyle D. Knight

For assessment of CFD capability in the prediction of the aerothermodynamic loading on a hypersonic shock wave boundary layer interaction (SWBLI) region, the numerical simulation of hypersonic laminar flow over a blunt cone flare configuration is performed using the perfect gas laminar Navier-Stokes equations. Computational results are compared with experimental data measured by Infrared Thermography technology from the US Air Force Research Lab’s Mach 6 Ludwieg Tube wind tunnel. Heat transfer data from the simulation agrees well with the experiment upstream of the SWBLI region but the separation zone is overpredicted in all computational cases, suggesting that the experimental data does not converge to steady state.
Acknowledgements

First, I want to sincerely thank my advisor, Professor Doyle D. Knight. He guided me to the area of CFD simulations and patience to my countless mistakes. He is the example of a researcher and taught us the importance of hard work and planning. I would like to express my gratitude to Dr. Nadia Kianvashrad, for her support and help in answering my questions.

I would like to thank my parents, Benchi Chen and Aihong Zhu. I’m the only child for my parents and left home over 10 years. I know they are concerned for me everyday but still support and encourage me to choose the way I like.

I would like to thank Yashesh Sakharikar and Partth Laad for their time, support, and camaraderie during the days spent in the lab in room B112.
Dedication

To my parents, Benchi Chen and Aihong Zhu.
# Table of Contents

Abstract .................................................................................. ii  
Acknowledgements ................................................................. iii  
Dedication ............................................................................... iv  
List of Tables ........................................................................ vii  
List of Figures .......................................................................... viii  

1. Introduction ........................................................................ 1  
   1.1. Hypersonic Flight .......................................................... 1  
   1.2. Shock-Wave/Boundary-Layer Interactions ......................... 5  

2. Description of Experiment ................................................... 10  
   2.1. AFRL Mach-6 Ludwieg Tube ........................................... 10  
   2.2. Blunt Nose Double Cone Experiments .............................. 12  

3. Methodology ....................................................................... 14  
   3.1. Introduction .................................................................. 14  
   3.2. Governing Equations .................................................... 15  
   3.3. Finite Volume Method .................................................. 16  
   3.4. Inviscid Flux Methods ................................................... 19  
      3.4.1. Roe’s Method ........................................................ 19  
      3.4.2. Van Leer’s Method ............................................... 24  
   3.5. Reconstruction ............................................................ 26  
   3.6. Limiters ....................................................................... 30  
      3.6.1. Van Albada’s Limiter ............................................ 32
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6.2. The Minimum Modulus (Min-Mod) Limiter</td>
<td>32</td>
</tr>
<tr>
<td>3.7. Viscous flux</td>
<td>32</td>
</tr>
<tr>
<td>3.8. Time Integration Methods</td>
<td>33</td>
</tr>
<tr>
<td>3.8.1. Steady State Simulation</td>
<td>33</td>
</tr>
<tr>
<td>3.8.2. Implicit Dual Time Scheme</td>
<td>33</td>
</tr>
<tr>
<td>3.9. Boundary Condition</td>
<td>34</td>
</tr>
<tr>
<td>3.10. Initial Condition</td>
<td>38</td>
</tr>
<tr>
<td>3.11. Grid Generation</td>
<td>39</td>
</tr>
<tr>
<td>3.12. Zonal Decomposition</td>
<td>41</td>
</tr>
<tr>
<td>4. Results</td>
<td>42</td>
</tr>
<tr>
<td>4.1. Convergence Study</td>
<td>43</td>
</tr>
<tr>
<td>4.2. Flow Patterns</td>
<td>47</td>
</tr>
<tr>
<td>4.3. Comparison with Experiment</td>
<td>52</td>
</tr>
<tr>
<td>4.3.1. Steady State Simulations</td>
<td>52</td>
</tr>
<tr>
<td>4.3.2. Time Accurate Simulations</td>
<td>53</td>
</tr>
<tr>
<td>4.3.3. Discussion</td>
<td>54</td>
</tr>
<tr>
<td>5. Conclusion</td>
<td>57</td>
</tr>
<tr>
<td>References</td>
<td>58</td>
</tr>
</tbody>
</table>
List of Tables

2.2. Simulation cases ................................................................. 13
3.1. Boundary conditions: Axisymmetric Line ............................... 37
3.2. Boundary conditions: Fixed at Q .............................................. 37
3.3. Boundary conditions: extrapolation ......................................... 38
3.4. Boundary conditions: isothermal, no-slip wall ......................... 38
3.5. Boundary conditions: Positive/Negative Axisymmetric Walls .... 38
3.6. Details of Grid ................................................................. 40
## List of Figures

1.1. LAPCAT A2 .............................................................. 1  
1.2. HTV-2 ........................................................................ 2  
1.3. HIFiRE 8 ................................................................... 3  
1.4. Cone/flare shock-wave/boundary-layer interaction schematic. [1] ............ 4  
2.3. AFRL cone/flare model geometry (dimensions are in mm) [1] ................... 12  
2.4. AFRL cone/flare model in test section [3] ............................. 12  
3.1. Roe’s solution to the General Riemann Problem [54] ............................... 23  
3.2. Boundary and first interior cell ........................................... 35  
3.3. Computational Domain .................................................... 35  
3.4. Q Spec Input ............................................................... 36  
3.5. Grid at cone/flare junction ............................................... 39  
3.6. Grid at nosetip .............................................................. 40  
4.1. Stanton number for Run 1 in 0.56M cells ............................... 43  
4.2. Stanton number for Run 1 in 1.12M cells ............................. 44  
4.3. Stanton number for Run 2 in 0.56M cells ............................. 45  
4.4. Stanton number for Run 2 in 1.12M cells ............................. 45  
4.5. Stanton number for Run 3 in 0.56M cells ............................. 46  
4.6. Stanton number for Run 3 in 1.12M cells ............................. 46  
4.7. Mach numbers of Steady State Simulation after 30000 steps in 0.56M grid. 47  
4.8. Mach numbers around nose of Steady State Simulation after 30000 steps in 0.56M grid. .................................................. 48
4.9. Mach numbers around flare of Steady State Simulation after 30000 steps in 0.56M grid. 

4.10. Mach numbers of Steady State Simulation after 250000 steps in 0.56M grid. 

4.11. Mach numbers of Time Accurate Simulation with Roe’s method after 0.05 s in 0.56M grid. 

4.12. Mach numbers of Time Accurate Simulation with Van Leer method after 0.05 s in 0.56M grid. 


4.14. Stanton Number before $x/L < 0.4$ in Run 1. 

4.15. Time Accurate simulation in 0.56M cells after 0.05 s. 

4.16. Time Accurate simulation in 1.12M cells after 0.05 s.
Chapter 1

Introduction

1.1 Hypersonic Flight

Renewed interest in hypersonic flight vehicles in civilian aviation and scientific applications has grown in recent years. The SpaceLiner is a long-term hypersonic passenger transport project developing at the German Aerospace Center since 2005. The SpaceLiner is aimed to cruise at Mach 9 or 20 to reduce 75% to 80% actual flight time compared to conventional subsonic airliner operation [4]. The ultra long-haul flight like Europe to Australia could be finished within 90 minutes by the SpaceLiner [5].

The 'Reaction Engines Limited LAPCAT Configuration A2' called the 'LAPCAT A2' is a hypersonic jet airliner design as part of the 'Long-Term Advanced Propulsion Concepts and Technologies' by British aerospace engineering. The objective of this program is developing a commercial transport aircraft with cruising speeds up to Mach 4 to reduce the duration of antipodal flights to less than 2 to 4 hours [6]. The LAPCAT A2 is shown in Fig. 1.1.

![LAPCAT A2](image)

Figure 1.1: LAPCAT A2

The 'High-Speed Experimental Fly Vehicles-INTernational' called the 'HEXAFLY-INT'
is a hypersonic civil transportation vehicle developing from the LAPCAT [7]. The goal of this project is achieving a cruise flight Mach number of 7 to 8 in a controlled way [8]. The HEXAFLY-INT would be able to take passengers from Brussels to Sydney in 2 hours and 55 minutes.

The natural follow-on project of previous series of European projects is the high speed passenger stratospheric flight 'STRATOFLY'. It is planned is to cruise at Mach number 8.0 at a stratospheric altitude [9].

The 'Zero Emission Hypersonic Transport' (ZEHST) is a hypersonic passenger airliner project by the multinational aerospace conglomerate EADS and the Japanese national space agency JAXA. The ZEHST would be capable to take 50-100 passengers from Tokyo to Los Angeles in less than 3 hours at a maximum speed of Mach 4.5 [10].

Projects related to hypersonic flight are not constrained to passenger transportation. The 'Force Application and Launch from CONtinental United States’ (FALCON) is a program between the Defense Advanced Research Project Agency (DARPA) and the United States Air Force (USAF) since 2003. The purpose of this program is developing and validating hypersonic technologies [11]. One aircraft design under this program was the 'Hypersonic Technology Vehicle' (HTV-2) and achieved Mach 20 in 2010 and 2011’s test flight. The figure of this HTV-2 is shown in Fig. 1.2 below. The Boeing X-51 Waverider vehicle is another flight demonstration of 'Hypersonic Technology Vehicle' program [12] designed for flight at Mach 5.0. Its test flight started in 2010.

Figure 1.2: HTV-2

The 'Sharp Edge Flight Experiment' (SHEFEX) is conducted by German Aerospace Center (DLR) since 2005. The first design SHEFEX I was tested in 2005 and the second
design SHEFEX II was tested in 2011 and reached Mach number over 11 [13].

The University of Queensland is working on several hypersonic projects since 2000. One program named the 'Scramjet Powered Accelerator for Reusable Technology Advancement' (SPARTAN) has five trajectory phases and would achieve Mach number 20.98 in phase 5 [14].

The 'Hypersonic International Flight Research Experimentation' (HIFiRE) is a joint program of Australian Department of Defense and the United States Air Force Flight Dynamics Laboratory to develop and validate technologies to hypersonic aerospace system since 2009 [15] [16]. The HIFiRE model reached Mach number 7.7-7.9 in the test [17]. The HIFiRE 8 is shown in Fig. 1.3

![HIFiRE 8](image)

Figure 1.3: HIFiRE 8

Avangard is a hypersonic glide vehicle developed in Russia. It was successfully tested twice in 2016 and 2018 and reaching Mach 20 [18]. The Angara family of launchers is under development by the Russian Federation [19]. China has tested DF-ZF Hypersonic Glide Vehicle (HGV) nine times since 2014 at Mach numbers between 5-10 [20].

For such hypersonic flight vehicles, analysis of aerothermodynamic loads (i.e., surface heat transfer and surface pressure) is essential especially for the interaction of shock waves with the vehicle boundary layers. In hypersonic flight, heat transfers from the boundary layer to the cooler vehicle surface. The separation of the boundary layer from the surface leads to a huge impact on pressure and heating distribution and shock wave/boundary layer
boundary layer interaction (SWBLI) is one common reason for boundary layer separation due to the high pressure region generated by an impinging shock.

SWBLI on an axisymmetric cone/flare model is illustrated in Fig. 1.4. The growing boundary layer faces an adverse pressure gradient generated by the flare and separates from the surface. The separation region moves upstream and forms the separation shock. The separated boundary layer will reattach downstream of the flare if the flare is long enough and will generate the attachment shock. Extremely high peak heat transfer will localize in the interaction region and potentially lead to structural failure by excessive heating.

![Cone/flare shock-wave/boundary-layer interaction schematic.][1]

One famous example of this was the unexpected trim angle on space shuttle flight STS-1. The body flap angle on STS-1 was designed to maintain 8° to 9° during reentry period but this angle extended to 14° in real flight. The postflight analysis found that the prediction of surface pressure distribution on space shuttle did not accurately consider the effect of shock wave boundary layer interaction generated by the body flap [21].

For all these hypersonic projects, experimental research with the wind tunnel and test flight is indispensable but such experiments are expensive and dangerous. Since 1970, computational fluid dynamics (CFD) became an important role. In 1971, Robert MacCormack first used CFD to solve Mach 2.0 flow in the two dimensional Navier Stokes equations [22]. In 1986, Joe Shang numerically solved a full Navier-Stokes equations for X-24C hypersonic vehicle at Mach 5.95 [23].
In these 40 years, several new algorithms have been published and improved the accuracy of the simulations. For example, two inviscid flux algorithm, Roe’s method and Van Leer’s method, were introduced in 1981 and 1997. The development of high performance computer clusters providing enormous fast processes and memory space enables researchers begin to simulate the phenomena that cannot imagined before. Several recent commercial software for hypersonic simulation enables more researchers take part in the CFD area.

In this Ph.D. dissertation, we choose the commercial software GASPex with several advance CFD methods to perform shock wave boundary layer interaction in a blunt cone flare model.

1.2 Shock-Wave/Boundary-Layer Interactions

The phenomenon of shock wave boundary layer interactions (SWBLI) has been studied for more than 70 years [24]. Most of early SWBLI studies employed experiments on simplified geometries and collected large sets of data for future assessment of CFD capability for accurate prediction in shock wave boundary layer interaction problems. During the past twenty years, more and more numerical studies were performed [25][26][27] and showed potential for accurate prediction of some flow features in the interaction region. However, numerical simulations have not consistently predicted peak heat transfer values in low and high enthalpy hypersonic flow within experimental uncertainly [19].

In experimental studies of SWBLI, the most documented cases are the two-dimensional interaction with compression ramp or double wedge. Grasso and Marini [28] conducted a series of two-dimensional numerical simulations of low enthalpy hypersonic flow past a compression ramp at Mach 14.1 using the Navier-Stokes equations for a perfect gas. An extensive study of low enthalpy flow at Mach numbers from 6 to 14.1 for a two-dimensional compression ramp was performed by Marini [29] using the same governing equations. The computed surface pressure, skin friction and Stanton number agreed with the experiments [29][30].

Olejniczak et al.[31] performed numerical and experimental studies of high enthalpy hypersonic flow past double wedge geometries in nitrogen with freestream velocities from 5.9 km/s to 6.3 km/s. Navier-Stokes equations with mass equation for each species (N2 and N)
and a separate vibrational energy equation were used in the numerical simulations. The size of the separation region was underpredicted by the computation. The heat transfer rate data in the separation region obtained from simulations agreed with experiments. However, the location of the peak heat transfer in the simulations was not consistent with the experiments. The reasons for disagreement include uncertainties in the dissociation rates, non-Boltzmann vibrational energy distributions in the freestream, and non-continuum formulations at the shock interaction region.

Reinartz et al.[32] numerically simulated the hypersonic flow over double wedge configurations at Mach 8.3 and 7.42 with stagnation temperature at 1420K and 2720K. Both numerical and experimental results showed agreement on the shape of the Stanton number distribution. However, the peak Stanton number values obtained from experiment were much higher than the laminar simulations suggesting a transition from laminar flow to turbulent flow over the separation region. The second fully turbulent simulation with two equation SSG (Speziale, Sarkar and Gatski) model was performed [33]. Results from fully turbulent simulations showed that the computed heat flux on the first wedge was greater than experiment but the peak heating values were close to experiment. The third simulation assumed laminar flow on the first and turbulent flow on the second wedge. The results of the combined laminar/turbulent simulations were closer to experiment than previous simulations.

NATO STO AVT Task Group 205 performed two-dimensional simulations of a double wedge at Mach number 7.1 with stagnation enthalpies ranging from 2.1 to 8.0 MJ/kg in nitrogen and air [34]. NATO STO AVT Task Group 205 focused on accessing CFD predictive capabilities for aerodynamic heating in hypersonic flow. Researchers compared their computational results with the measurements from double wedge experiments conducted by Swantek and Austin in the Hypervelocity Expansion Tube at the University of Illinois Urbana-Champaign [35]. In this group, researchers from CIRA performed steady state two-dimensional simulations and several researchers performed two dimensional time-accurate simulations [36], while Komives et al.[37] and Reinert et al.[38] conducted three dimensional simulations. Three-dimensional simulations showed reasonable agreement with the experiments and indicated that the flow in the experiment was three-dimensional. Moreover,
the heat transfer profile collected from steady state two-dimensional simulations displayed significant difference with experiment.

A number of experiments investigated the flowfield of three-dimensional or axisymmetric geometries which are closer to realistic hypersonic flight. Chanetz et al. [39] performed experiments and numerical studies of shock wave boundary interaction on a hollow cylinder flare geometry in the low enthalpy hypersonic laminar flow at Mach number 10. Three Navier-Stokes codes and one Direct Simulation Monte-Carlo code were used in the numerical simulations. Results from the three Navier-Stokes simulations showed agreement on surface pressure and heat flux with experiments, while only slightly overpredicted the separation region length and pressure level after reattachment. However, simulation results from the DSMC code were consistent as the Navier-Stokes codes. DSMC overpredicted the peak pressure on the flare by approximately 50%. Mortazavi and Knight [40] conducted the same simulation in Navier-Stokes code with a finer grid, and the simulation results were consistent with the experiments mentioned above.

Gaitonde [41] simulated Mach 9.5 flow past a 25/55 degree sharp double cone with the Navier-Stokes equations under perfect gas assumption. Comparison with experimental data showed good agreement on surface heat transfer. The difference between computational and experimental [42][43] heat transfer rates was within 15% of the maximum values. Additional simulations showed that variations in air or nitrogen, freestream and wall temperatures had a modest effect on the simulation results.

Druguet et al. [44] studied the effects of the numerics on the simulation of hypersonic flow past a sharp double cone (same 25/55 degree model as mentioned above) in air at Mach 11.3 and a stagnation enthalpy of 3.7 MJ/kg. Navier-Stokes simulations under perfect gas assumption were performed. Five different inviscid flux algorithms and four inviscid flux limiters were examined, respectively. The surface pressure and heat transfer predicted by highly resolved grids showed good agreement with experimental data. The least dissipative schemes showed better performance on predicting accurate results on a coarser grid.

Researchers in US and Europe from RTO AVT 136 conducted a series of independent computations of double cone flow and compared with experimental data to examine CFD software capability to predict hypersonic shock wave laminar boundary layer interactions.
Experiments were performed at CUBRC for the 25/55 degree sharp double cone in nitrogen at Mach 11.5 and stagnation enthalpies of 5.38 MJ/kg and 9.17 MJ/kg. For the high enthalpy case (Run 42), computational surface pressure and heat transfer from six researchers agreed well with experiments. For the low enthalpy case (Run 40), simulations and experimental data had significant discrepancy. The Run 40 experiment showed steady flow, while an unsteadiness in the flowfield was observed by six independent numerical simulations. To access the effect of Reynolds number, an additional experiment was performed with the same enthalpy as Run 40 but half the Reynolds number in Run 40. Both experiments and simulations reached steady state and the computed surface pressure and heat transfer showed close agreement with experiment.

Most double cone models have a sharp nose. However, the leading edge regions of hypersonic flight vehicles are generally blunted in practical applications. Borovoy et al. investigated the heat transfer of shock wave boundary layer interaction on varying bluntness plates at Mach number from 5 to 10 and Reynolds numbers from $0.3 \times 10^6/m$ to $20 \times 10^6/m$ by experiments and numerical simulations. Experimental results showed that increasing nose radius dramatically reduces the peak Stanton number in the reattachment region by increasing separation length and decreasing gas density in the high entropy layer. Results of numerical simulation showed agreement on qualitative features of the flow structure in the interaction region; however, the numerical predicted separation length had consideration discrepancy with the experiments.

Jiaao Hao et al. performed a numerical simulations of hypersonic shock wave laminar boundary layer interaction over 25/55 degree double with various nose radii with a Mach number at 9.87 and stagnation enthalpy of 5MJ/kg. Non-equilibrium Naiver-Stokes equations were utilized in the simulations. Numerical surface pressure and heat flux were compared with the experiments from Run 31 in Holden et al. The length of separation region, surface pressure and heat flux were significantly reduced with increasing bluntness of nose.

In summary, CFD methods have the capability to predict shock wave boundary layer interaction in hypersonic flow but cannot consistently predict the surface pressure, heat
transfer and length of the separation zone accurately. The motivation of this dissertation is that Running et al.[1] performed infrared-thermography measurements and provided valuable global contours of the SWBLI. Thus experimental data can be compared with computational results. The objective of my Ph.D. research is to simulate the experiment of Running et al.[1] and compare with the experimental results.
Chapter 2

Description of Experiment

The numerical simulations of shock wave boundary layer interaction in this dissertation are compared with hypersonic flow over a blunt double cone experiments performed by Running et al.[49]. These experiments measured surface heat transfer through non-intrusive infrared-thermography. Infrared-thermography measurements provide global contours of the SWBLI phenomenon which can select as boundary conditions or surface results to compare with computations.

2.1 AFRL Mach-6 Ludwieg Tube

The experiment data were collected in the Mach 6 Ludwieg Tube wind tunnel at the Air Force Research Laboratory (AFRL) as shown in Fig. 2.1 below. This is a conventional noise wind tunnel equipped with a 30 inch diameter Mach 6 nozzle and powered by two compressors and two vacuum pumps. The start of the tunnel is controlled by a plug-type fast valve in the contraction exit [2]. Two periods of approximately 100 ms steady flow are contained in each test and the heat transfer data in this experiment was collected in the first period of steady flow [49].
As for the Mach number at the test region, engineers at the AFRL performed tunnel characterization through a pitot probe rake. The figure of the pitot probe rake is shown in Fig. 2.2. Based on the pitot measurement, the Mach number was 6.14 within 200 mm radius circle region around the core [3]. The tunnel performs hypersonic flow tests at three initial stagnation pressures. Table 2.1 introduces the test flow conditions calculated by isentropic flow relations and Sutherland’s viscosity law for the first period steady flow.
<table>
<thead>
<tr>
<th>Conditions</th>
<th>$M_\infty$</th>
<th>$P_0$ (kPa)</th>
<th>$T_0$ (K)</th>
<th>$R_\infty$ ($10^6$/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6.14</td>
<td>920 ± 6.8</td>
<td>490 ± 5</td>
<td>7.6 ± 0.2</td>
</tr>
<tr>
<td>2</td>
<td>6.14</td>
<td>1224 ± 7.3</td>
<td>490 ± 5</td>
<td>10.1 ± 0.2</td>
</tr>
<tr>
<td>3</td>
<td>6.14</td>
<td>2427 ± 6.8</td>
<td>490 ± 5</td>
<td>20.0 ± 0.2</td>
</tr>
</tbody>
</table>

Table 2.1: Flow Conditions for the test flow [1]

2.2 Blunt Nose Double Cone Experiments

The cone/flare model is shown in Fig. 2.3 and Fig. 2.4. The half angle of the first circular cone is a constant 7 degrees and the diameter at cone/flare junction is 148 mm. Four varying nose tip radii and four different flare angles $\theta_2$ are introduced in the experiments. The four nose radii are nominally sharp, 0.5 mm, 5.1 mm and 10.2 mm and four flare angles are 34 degree, 37 degree, 40 degree and 43 degree [1]. As shown in Fig. 2.3, the length of the first cone would slightly decrease after installing a blunt nose. The model surface is isothermal at 297K.

![AFRL cone/flare model geometry (dimensions are in mm) [1]](image1)

![AFRL cone/flare model in test section [3]](image2)
The steady state surface temperature of the cone/flare model was captured by an InfraTec 8300 hp infrared camera and filtered by 0.014s (5 frames). The surface heat flux at the wall was computed by inputting the infrared temperature data into the FORTRAN QCALC code. The uncertainty of Stanton number is estimated at ±15% [49].

The flowfield for test flow condition 1 in Table 2.1 over 10.2 mm nose double cone with 37 degree flare was steady and laminar according to experimental data [1]. This case is selected for the simulation case using the commercial CFD code GASPex [50] and three numerical runs are designed as shown in Table 2.2 below. Run 1 uses steady state simulation with Van Leer’s method and Min-Mod limiter, Run 2 approaches a steady state solution through time-accurate simulations with Roe’s method and Van Albada limiters and Run 3 performs time-accurate simulations with Van Leer method and Min-Mod limiter.

<table>
<thead>
<tr>
<th>Run</th>
<th>Inviscid Flux</th>
<th>Limiter</th>
<th>Time Integration Methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Van Leer’s</td>
<td>Min Mod</td>
<td>Steady State</td>
</tr>
<tr>
<td>2</td>
<td>Roe’s</td>
<td>Van Albada</td>
<td>Dual Time Stepping</td>
</tr>
<tr>
<td>3</td>
<td>Van Leer’s</td>
<td>Min Mod</td>
<td>Dual Time Stepping</td>
</tr>
</tbody>
</table>

Table 2.2: Simulation cases
Chapter 3
Methodology

Numerical simulations in this dissertation used the commercial flow solver GASPex. The methods used in this GASPex are described including the governing equations, flux algorithms, reconstruction methods and time integration techniques.

3.1 Introduction

The first step to solve the problem is selecting the correct set of governing equations. The next step is discretizing the governing equations. For hypersonic problems, the discontinuity of the conservative variables would occur in the adjacent cells which means it is necessary to carefully calculate the flux at the faces and reconstruction methods for specific accuracy are required. Then, it is necessary to choose steady-state or time-accurate simulations to solve the problem.

In this chapter, the governing equations are described in Section 3.2. The finite volume method is first introduced in Section 3.3. In Section 3.4, the two inviscid flux methods used to calculate the inviscid flux at the cell faces, Roe’s method and Van Leer’s method, are described. For the flux calculations, the values of the primitive variables at left side and right side of each faces are estimated by reconstruction methods. Therefore, the reconstruction method MUSCL is introduced in Section 3.5 and limiter is described in Section 3.6. The method to calculate the viscous flux is described in Section 3.7. Then, time integration methods such as dual time stepping method steady state method are introduced in Section 3.8.

In the numerical simulations, the correct boundary conditions should be applied to maintain a stable simulation and prevent un-physical phenomenon in the simulations. The
boundary conditions such as axisymmetric, fixed, no-slip isothermal, the first order extrapolation and axisymmetric wall are introduced in Section 3.9 and the initial condition is covered in Section 3.10.

Grid generation is described in Section 3.11. In Section 3.12, zonal decomposition is introduced which used to separate entire computational domain into several smaller part then corporate with the message passing interface (MPI) to improve the calculation efficiency.

### 3.2 Governing Equations

Choosing the correct governing equations is the first step to solve the problem. Rules for the best governing equations is to include all the important aspects of the problem and ignore unnecessary physics model to simplify the solving process. In this dissertation, the laminar Naiver-Stokes equations are selected because from the experimental data, the entire flowfield is laminar flow. Calorically perfect assumption is made at here because the local maximum temperature never exceeds $490K$ [1] which is insufficient to dissociate even oxygen. Therefore, the laminar Navier-Stokes equations for a perfect gas are:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \tag{3.1}
\]

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \tag{3.2}
\]

\[
\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial (\rho \varepsilon + p) u_j}{\partial x_j} = -\frac{\partial q_j}{\partial x_j} + \frac{\partial (u_i \tau_{ij})}{\partial x_j} \tag{3.3}
\]

\[
p = \rho RT \tag{3.4}
\]

where $\rho$ is the fluid density, $p$ is the fluid static pressure, $u_j$ is the velocity vector, and $\tau_{ij}$ is the compressible viscous stress tensor:

\[
\tau_{ij} = -\frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{3.5}
\]

where $\varepsilon$ is the total energy per unit mass:

\[
\varepsilon = e + \frac{1}{2} u_i u_i \tag{3.6}
\]

and $e$ is the internal energy per unit mass:

\[
e = c_v T \tag{3.7}
\]
and $q_j$ is the heat flux vector which are defined as:

$$q_j = -k \frac{\partial T}{\partial x_j}$$

where the dynamic viscosity $\mu$ is defined by Sutherland’s Law:

$$\mu = \mu_0 \left( \frac{T}{T_0} \right)^{3/2} \frac{T_0 + S}{T + S}$$

and molecular Prandtl number $Pr = \mu C_p / k$ is 0.72. $c_v$, $T$ and $k$ are the specific heat at constant volume, static temperature, thermal conductivity. The gas constant of air is 287 J/kg·K.

### 3.3 Finite Volume Method

In order to evaluate the governing equations, GASPex invokes the finite volume method to discretize the spatial and temporal domains. The computational domain is divided into a finite number of control volumes to evaluate the solution. The partial differential equations for a three-dimensional flow of a fluid with equilibrium chemistry and internal energy can be written in integral form as:

$$\frac{\partial}{\partial t} \iiint Q dV + \oint_A \left( F(Q) \cdot \hat{n} \right) dA = 0$$

(3.9)

The conserved quantities are denoted by $Q$, the flux vector by $F$. The vector $\hat{n}$ represents the unit normal vector at a cell face, denoted positive when pointing outward from the cell. After denoting the cell volume as $Vol$ and the area of each cell face as $\Delta A$, then we can rewrite eqn.3.9 exactly as

$$Vol \frac{\partial Q}{\partial t} + \oint_A \left( F(Q) \cdot \hat{n} \right) dA = 0$$

(3.10)

where the cell average of the conserved-variable field is defined as [50]

$$\bar{Q} \equiv \frac{1}{Vol} \iiint Q dV$$

(3.11)
In GASPex, the Equation (3.10) can be approximated on an arbitrarily shape finite volume as

$$\text{Vol} \left( \frac{\partial Q}{\partial q} \right) \frac{\partial q}{\partial t} + \sum_A (F \cdot \hat{n}) \Delta A = 0 \quad (3.12)$$

The formulation above can be applied to the governing equations for the compressible laminar Navier-Stokes equations for a perfect gas and rewrite in the vector form as:

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} = \frac{\partial R}{\partial x} + \frac{\partial S}{\partial y} + \frac{\partial T}{\partial z} \quad (3.13)$$

where

$$Q = \begin{pmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \\ Q_5 \end{pmatrix} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho e \end{pmatrix} \quad (3.14)$$

Then, the vectors $E$, $F$, and $G$ are inviscid flux components in the $x$, $y$, and $z$ directions, respectively.

$$E = \begin{pmatrix} E_1 \\ E_2 \\ E_3 \\ E_4 \\ E_5 \end{pmatrix} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u w \\ (\rho e + p) u \end{pmatrix} \quad (3.15)$$

$$F = \begin{pmatrix} F_1 \\ F_2 \\ F_3 \\ F_4 \\ F_5 \end{pmatrix} = \begin{pmatrix} \rho v \\ \rho v u \\ \rho v^2 + p \\ \rho v w \\ (\rho e + p) v \end{pmatrix} \quad (3.16)$$
\[
G = \begin{pmatrix}
G_1 \\
G_2 \\
G_3 \\
G_4 \\
G_5
\end{pmatrix} = \begin{pmatrix}
\rho w \\
\rho w u \\
\rho w v \\
\rho w^2 + p \\
(\rho e + p) w
\end{pmatrix}
\]

where \(u, v, \) and \(w\) denote the velocity components in \(x,y\) and \(z\) directions, \(\rho\) is the fluid density, \(p\) is the fluid pressure, and \(e\) is the internal energy per unit mass.

The vectors \(R, S,\) and \(T\) are viscous flux components in the \(x, y,\) and \(z\) directions.

\[
R = \begin{pmatrix}
R_1 \\
R_2 \\
R_3 \\
R_4 \\
R_5
\end{pmatrix} = \begin{pmatrix}
0 \\
\tau_{xx} \\
\tau_{yx} \\
\tau_{zx} \\
\tau_{xx} u + \tau_{xy} v + \tau_{xz} w - q_x
\end{pmatrix}
\]

\[
S = \begin{pmatrix}
S_1 \\
S_2 \\
S_3 \\
S_4 \\
S_5
\end{pmatrix} = \begin{pmatrix}
0 \\
\tau_{xy} \\
\tau_{yy} \\
\tau_{yz} \\
\tau_{xy} u + \tau_{yy} v + \tau_{yz} w - q_y
\end{pmatrix}
\]

\[
T = \begin{pmatrix}
T_1 \\
T_2 \\
T_3 \\
T_4 \\
T_5
\end{pmatrix} = \begin{pmatrix}
0 \\
\tau_{xz} \\
\tau_{yz} \\
\tau_{zz} \\
\tau_{xz} u + \tau_{yz} v + \tau_{zz} w - q_z
\end{pmatrix}
\]

In the viscous vectors above, \(q_i\) is the heat transfer vector and \(\tau_{ij}\) is the viscous shear stress.
3.4 Inviscid Flux Methods

In the hypersonic flow simulations, the discontinuity of the conservative variable would occur in the adjacent cells, and thus it is important to use some methods to calculate the inviscid flux at the interface around shock discontinuities. Several methods can be used to calculate the inviscid flux at the interface. The Flux Difference Splitting Methods (known as Godunov, Riemann) use approximate solutions of the Riemann problem, while Flux Vector Splitting Methods construct flux at the interface based on the direction of the characteristic signal. Roe’s [51][52] and Van Leer’s [53] methods are used for simulations in this dissertation. Roe’s method is a Godunov method while Van Leer’s method is flux vector splitting method. In this section, derivations of inviscid flux are based on the one-dimensional perfect gas flow and the extension to three-dimensional flows is straightforward.

3.4.1 Roe’s Method

Consider the one-dimensional Euler equations:

\[
\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} = 0 \tag{3.22}
\]

where

\[
Q = \begin{bmatrix}
\rho \\
\rho u \\
\rho e
\end{bmatrix} \quad F = \begin{bmatrix}
\rho u \\
\rho u^2 + p \\
u (\rho e + p)
\end{bmatrix} \tag{3.23}
\]

where,

\[
\rho e = \frac{p}{\gamma - 1} + \frac{1}{2} \rho u^2 \tag{3.24}
\]
and the specific total energy is
\[ e = H - \frac{p}{\rho} \] (3.25)
where \( H \) is the total enthalpy per unit mass.

We can rewrite Euler equations as:
\[ \frac{\partial Q}{\partial t} + A \frac{\partial Q}{\partial x} = 0 \] (3.26)
where \( A \) is the Jacobian:
\[
A(Q) = \begin{pmatrix}
0 & 1 & 0 \\
(\gamma - 3) u^2/2 & (3 - \gamma) u & \gamma - 1 \\
-Hu + (\gamma - 1) u^3/2 & H - (\gamma - 1) u^2 & \gamma u
\end{pmatrix}
\] (3.27)

Roe constructed an approximate form of the Euler equations:
\[ \frac{\partial Q}{\partial t} + \tilde{A}(Q_l, Q_r) \frac{\partial Q}{\partial x} = 0 \] (3.28)
where assuming \( \tilde{A}(Q_l, Q_r) \) is a constant matrix consisted of left state \( Q_l \) and right state \( Q_r \). The matrix \( \tilde{A} \) is an approximation of \( A \) and satisfies the following four properties [51].

1. \( \tilde{A} \) provides a linear mapping from the vector space of \( Q \) to the vector space of \( F \).
2. \( \tilde{A}(Q_l, Q_r) \to \tilde{A}(Q) \) as \( Q_l \to Q_r \to Q \).
3. For any \( Q_r \) and \( Q_l \), \( \tilde{A}(Q_l, Q_r) \times (Q_l - Q_r) \equiv F_l - F_r \).
4. The eigenvectors of \( \tilde{A}(Q_l, Q_r) \) are linearly independent.

In order to get matrix \( \tilde{A} \), We have a parameterization vector \( \nu \) as
\[
\nu = \begin{bmatrix}
\nu_1 \\
\nu_2 \\
\nu_3
\end{bmatrix} = \begin{bmatrix}
\sqrt{\rho} \\
\sqrt{\rho u} \\
\sqrt{\rho H}
\end{bmatrix}
\] (3.29)

Vectors \( Q \) and \( F \) can be rewritten as
\[
Q = \begin{bmatrix}
\nu_1^2 \\
\nu_1 \nu_2 \\
\frac{1}{\gamma} \nu_1 \nu_3 + \frac{\gamma - 1}{2 \gamma} \nu_2^2
\end{bmatrix} \quad F = \begin{bmatrix}
\nu_1 \nu_2 \\
\frac{\gamma - 1}{\gamma} \nu_1 \nu_3 + \frac{\gamma + 1}{2 \gamma} \nu_2^2 \\
\nu_2 \nu_3
\end{bmatrix}
\] (3.30)
\( Q \) and \( F \) are quadratic relative to the vector \( \nu \). Thus, it is possible to find matrix \( B \) and \( C \) such that

\[
\Delta Q = B \Delta \nu \\
\Delta F = C \Delta \nu
\]

(3.31)

(3.32)

where \( \Delta (\bullet) = (\bullet)_l - (\bullet)_r \). The matrix \( B \) and \( C \) can be found respectively.

\[
B = \begin{bmatrix}
2\nu_1 & 0 & 0 \\
\nu_2 & \nu_1 & 0 \\
\frac{1}{\gamma} \nu_3 & \frac{\gamma-1}{\gamma} \nu_2 & \frac{1}{\gamma} \nu_1
\end{bmatrix}
\]

(3.33)

\[
C = \begin{bmatrix}
\nu_2 & \nu_1 & 0 \\
\frac{\gamma-1}{\gamma} \nu_3 & \frac{\gamma+1}{\gamma} \nu_2 & \frac{\gamma-1}{\gamma} \nu_1 \\
0 & \nu_3 & \nu_2
\end{bmatrix}
\]

(3.34)

where \( \tilde{\nu} \equiv \frac{1}{2} (\bullet_l + \bullet_r) \).

Thus,

\[
\Delta F = A \Delta Q \\
\Delta \nu = C^{-1} AB \Delta \nu \\
A = CB^{-1}
\]

(3.35)

(3.36)

(3.37)

(3.38)

The matrix \( \tilde{A} \) is [54]:

\[
\tilde{A} = \left\{ \begin{array}{ccc}
0 & 1 & 0 \\
\frac{(\gamma-3)}{2} \left( \frac{\nu_2}{\nu_1} \right)^2 & (3-\gamma) \frac{\nu_2}{\nu_1} & \gamma - 1 \\
-\frac{\nu_2 \nu_3}{\nu_1^2} + \frac{\gamma-1}{2} \left( \frac{\nu_2}{\nu_1} \right)^3 & \left( \frac{\nu_2}{\nu_1} \right) (\gamma - 1) \left( \frac{\nu_3}{\nu_1} \right)^2 & \gamma \left( \frac{\nu_2}{\nu_1} \right)
\end{array} \right\}
\]

(3.39)

The simplified matrix \( \tilde{\tilde{A}} \) is

\[
\tilde{\tilde{A}} = \left\{ \begin{array}{ccc}
0 & 1 & 0 \\
(\gamma - 3) \tilde{u}^2/2 & (3-\gamma) \tilde{u} & \gamma - 1 \\
-\tilde{H} \tilde{u} + (\gamma - 1) \tilde{u}^3/2 & \tilde{H} - (\gamma - 1) \tilde{u}^2 & \gamma \tilde{u}
\end{array} \right\}
\]

(3.40)
where:
\[
\tilde{u} \equiv \frac{p_l}{\rho_l} = \frac{\sqrt{\rho_l u_l + \sqrt{\rho_l} u_r}}{\sqrt{\rho_l} + \sqrt{\rho_r}} \tag{3.41}
\]
\[
\tilde{H} \equiv \frac{p_l}{\rho_l} = \frac{\sqrt{\rho_l H_l + \sqrt{\rho_l} H_r}}{\sqrt{\rho_l} + \sqrt{\rho_r}} \tag{3.42}
\]

Here $\tilde{u}$ is the Roe-averaged velocity and $\tilde{H}$ is the Roe-averaged total enthalpy. The matrix $\tilde{A}(Q_l, Q_r)$ is called the Roe matrix.

The eigenvalues $\tilde{\lambda}_i$ and the right eigenvectors $\tilde{e}_i$ of the vector $\tilde{A}$ can be directly found as:
\[
\tilde{\lambda}_1 = \tilde{u}, \tag{3.43}
\]
\[
\tilde{\lambda}_2 = \tilde{u} + \tilde{a}, \tag{3.44}
\]
\[
\tilde{\lambda}_3 = \tilde{u} - \tilde{a} \tag{3.45}
\]

The corresponding eigenvectors for this eigenvalues of matrix $\tilde{A}$ are
\[
\tilde{e}_1 = \begin{bmatrix} 1 \\ \tilde{u} \\ \frac{1}{2} \tilde{u}^2 \end{bmatrix}, \quad \tilde{e}_2 = \begin{bmatrix} 1 \\ \tilde{u} + \tilde{a} \\ \tilde{H} + \tilde{u} \tilde{a} \end{bmatrix}, \quad \tilde{e}_3 = \begin{bmatrix} 1 \\ \tilde{u} - \tilde{a} \\ \tilde{H} - \tilde{u} \tilde{a} \end{bmatrix} \tag{3.46}
\]
where $\tilde{a}$ is the speed of sound based on the Roe-averaged total enthalpy and Roe-averaged velocity and is given by:
\[
\tilde{a} = \sqrt{(\gamma - 1)(\tilde{H} - \frac{1}{2} \tilde{u}^2)} \tag{3.47}
\]

The Roe matrix can be diagonalized as
\[
\tilde{A}(Q_l, Q_r) = \tilde{S} \tilde{\Lambda} \tilde{S}^{-1} \tag{3.48}
\]
where $\tilde{S}$ is the matrix of right eigenvectors of $\tilde{A}(Q_l, Q_r)$.

\[
\tilde{S} = \begin{bmatrix} 1 & 1 & 1 \\ \tilde{u} & \tilde{u} + \tilde{a} & \tilde{u} - \tilde{a} \\ \frac{1}{2} \tilde{u}^2 & \tilde{H} + \tilde{u} \tilde{a} & \tilde{H} - \tilde{u} \tilde{a} \end{bmatrix} \tag{3.49}
\]
and:
\[
\tilde{S}^{-1} = \begin{bmatrix} 1 - (\gamma - 1)\tilde{u}^2/2\tilde{a}^2 & (\gamma - 1)\tilde{u}/\tilde{a}^2 & -(\gamma - 1)/\tilde{a}^2 \\ (\gamma - 1)\tilde{u}^2/4\tilde{a}^2 - \tilde{u}/2\tilde{a} & -(\gamma - 1)\tilde{u}/2\tilde{a}^2 + 1/2\tilde{a} & (\gamma - 1)/2\tilde{a}^2 \\ (\gamma - 1)\tilde{u}^2/4\tilde{a}^2 + \tilde{u}/2\tilde{a} & -(\gamma - 1)\tilde{u}/2\tilde{a}^2 - 1/2\tilde{a} & (\gamma - 1)/2\tilde{a}^2 \end{bmatrix} \tag{3.50}
\]
Knowing that \( \tilde{A} \) is assumed to be a constant, eqn (3.28) can be multiplied by \( \tilde{S}^{-1} \) to get:

\[
\frac{\partial R}{\partial t} + \tilde{\Lambda} \frac{\partial R}{\partial x} = 0 \quad (3.51)
\]

where:

\[
R \equiv \tilde{S}^{-1} Q = \begin{cases} R_1 \\ R_2 \\ R_3 \end{cases}
\]

and \( \tilde{\Lambda} \) is given by:

\[
\tilde{\Lambda} = \begin{cases} \tilde{\lambda}_1 & 0 & 0 \\ 0 & \tilde{\lambda}_2 & 0 \\ 0 & 0 & \tilde{\lambda}_3 \end{cases}
\]

(3.53)

The solution of eqn (3.51) is:

- \( R_1 \) = constant on curve \( C_1 \) defined by \( \frac{dx}{dt} = \tilde{\lambda}_1 = \tilde{u} \).
- \( R_2 \) = constant on curve \( C_2 \) defined by \( \frac{dx}{dt} = \tilde{\lambda}_1 = \tilde{u} + \tilde{a} \).
- \( R_3 \) = constant on curve \( C_3 \) defined by \( \frac{dx}{dt} = \tilde{\lambda}_1 = \tilde{u} - \tilde{a} \).

\( C_1, C_2, \) and \( C_3 \) are the characteristic curves of 3.51. The solution for \( R_1, R_2 \) and \( R_3 \) are shown below in Fig. 3.1.

![Diagram showing characteristic curves]

Figure 3.1: Roe’s solution to the General Riemann Problem [54]

Therefore,

\[
P_{k}^{n+1} = \frac{1}{2} (R_{kl} + R_{kr})^n + \frac{1}{2} \text{sign} \left( \lambda_k \right) (R_{kl} + R_{kr})^n
\]

(3.54)
where \( k = 1, 2, 3, r \) and \( l \) are right and left face values after reconstruction, and

\[
\text{sign} (\lambda_k) = \begin{cases} 
+1 & \lambda_k > 0 \\
0 & \lambda_k = 0 \\
-1 & \lambda_k < 0 
\end{cases}
\]  

(3.55)

Consider the semi-discrete form of the Euler equations:

\[
\frac{dQ_i}{dt} + \frac{F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}}{\Delta x} = 0
\]  

(3.56)

From definition of Roe matrix and eqn (3.48), the flux \( F_{i+\frac{1}{2}} \) is:

\[
F_{i+\frac{1}{2}} = (AQ)_{i+\frac{1}{2}} = AQ_{i+\frac{1}{2}} = (\bar{S}\bar{\Lambda}\bar{S}^{-1}) Q_{i+\frac{1}{2}}
\]  

(3.57)

From eqn (3.52), eqn (3.57) turns into:

\[
F_{i+\frac{1}{2}} = (\bar{S}\bar{\Lambda}\bar{S}^{-1}) \left( \bar{S}R \right)_{i+\frac{1}{2}} = \bar{S}\bar{\Lambda}R_{i+\frac{1}{2}}
\]  

(3.58)

Therefore,

\[
F_{i+\frac{1}{2}} = (R_l + R_r) + \frac{1}{2} \bar{S} |\bar{\Lambda}| (R_l + R_r)
\]  

(3.59)

Using \( Q \) to express \( R \):

\[
F_{i+\frac{1}{2}} = \left[ \bar{S}\bar{\Lambda}\bar{S}^{-1} (Q_l + Q_r) + \bar{S}\bar{\Lambda}\bar{S}^{-1} (Q_l - Q_r) \right]
\]  

(3.60)

The final form of inviscid flux \( F_{i+\frac{1}{2}} \) is given by:

\[
F_{i+\frac{1}{2}} = \frac{1}{2} \left[ F_l + F_r + \bar{S} |\bar{\Lambda}| \bar{S}^{-1} (Q_{i+\frac{1}{2}}^l - Q_{i+\frac{1}{2}}^r) \right]
\]  

(3.61)

### 3.4.2 Van Leer’s Method

Consider the one-dimensional Euler equations:

\[
\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} = 0
\]  

(3.62)

The flux vector \( F \) can be written:

\[
F = \begin{bmatrix} \rho a M \\ \frac{\rho a^2}{\gamma} (\gamma M^2 + 1) \\ \rho a^3 M \left( \frac{1}{(\gamma-1)} + \frac{1}{2} M^2 \right) \end{bmatrix}
\]  

(3.63)
In Van Leer’s method, the terms in eqn (3.63) including the Mach number $M$ is split into two parts. Density $\rho$ and the speed of sound $a$ are estimated using primitive variables at the left ($l$) and right side ($r$) of each faces. For the mass flux, the term involving the Mach number is simply $M$ and is split according to

$$M = M^+ + M^-$$  \hspace{1cm} (3.64)

The mass flux is:

$$\rho u = \rho_l a_l M^+ + \rho_r a_r M^-$$  \hspace{1cm} (3.65)

Where

$$M^+ = \begin{cases} 
0 & M \leq -1 \\
 f_1^+ & -1 \leq M \leq 1 \\
 M & M \geq 1 
\end{cases}$$  \hspace{1cm} (3.66)

And

$$M^- = \begin{cases} 
0 & M \leq -1 \\
 f_1^- & -1 \leq M \leq 1 \\
 0 & M \geq 1 
\end{cases}$$  \hspace{1cm} (3.67)

$M$ is the average Mach number at the interface

$$M = \frac{u_l + u_r}{a_l + a_r}$$  \hspace{1cm} (3.68)

For mass flux:

$$\rho u = \begin{cases} 
\rho_r a_r M & M \leq -1 \\
 \rho_l a_l f_1^+ + \rho_r a_r f_1^- & -1 \leq M \leq 1 \\
 \rho_l a_l M & M \geq 1 
\end{cases}$$  \hspace{1cm} (3.69)

Then,

$$f_1^+ = \frac{1}{4} (M + 1)^2$$

$$f_1^- = -\frac{1}{4} (M - 1)^2$$  \hspace{1cm} (3.70)

For the momentum flux:

$$\rho u^2 + p = \begin{cases} 
\gamma^{-1} \rho_r a_r^2 (\gamma M^2 + 1) & M \leq -1 \\
\gamma^{-1} \rho_r a_r^2 f_2^- + \gamma^{-1} \rho_l a_l^2 f_2^+ & -1 \leq M \leq 1 \\
\gamma^{-1} \rho_l a_l^2 (\gamma M^2 + 1) & M \geq 1 
\end{cases}$$  \hspace{1cm} (3.71)
Where:

\[ f_2^+ = \frac{1}{4} (M + 1)^2 [(\gamma - 1) M + 2] \]
\[ f_2^- = -\frac{1}{4} (M - 1)^2 [(\gamma - 1) M - 2] \]  

(3.72)

For the energy flux:

\[
(\rho e + p) u = \begin{cases} 
\rho_r a_3^2 M \left[ (\gamma - 1)^{-1} + \frac{1}{2} M^2 \right] & M \leq -1 \\
\rho_r a_3^2 f_3^- + \rho_l a_3^2 f_3^+ & -1 \leq M \leq 1 \\
\rho_l a_3^2 M \left[ (\gamma - 1)^{-1} + \frac{1}{2} M^2 \right] & M \geq 1 
\end{cases}
\]  

(3.73)

Where:

\[ f_3^+ = \frac{1}{8} (\gamma + 1)^{-1} (\gamma - 1)^{-1} (M + 1)^2 [(\gamma - 1) M + 2] \]
\[ f_3^- = -\frac{1}{8} (\gamma + 1)^{-1} (\gamma - 1)^{-1} (M - 1)^2 [(\gamma - 1) M - 2] \]  

(3.74)

### 3.5 Reconstruction

To evaluate the flux, we need to know the primitive variables (\(Q\)) at the cell faces. In the finite volume method, the value of \(Q\) is stored at the center of the cell. In order to estimate the value of \(Q\) at each face, reconstruction methods are needed to provide the link between the cell averages and the cell-face data.

Consider the semi-discrete form of the Euler equations:

\[
\frac{dQ_i}{dt} + \frac{(F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}})}{\Delta x} = 0 
\]

(3.75)

where \(Q_i\) is the average of depend variable vector over the cell, can be express as

\[ Q_i(t) = \frac{1}{V_i} \int_{V_i} Q dx dy dz \]  

(3.76)

and \(F_{i\pm\frac{1}{2}}\) are given by

\[ F_{i\pm\frac{1}{2}} = \frac{1}{A_{i\pm\frac{1}{2}}} \int_{x_{i\pm\frac{1}{2}}} \mathcal{F} dy dz \]  

(3.77)

where the area of faces at \(x_{i\pm\frac{1}{2}}\) is \(A_{i\pm\frac{1}{2}} = \Delta y \Delta z\).

The values of dependent variables at the left and right sides of each face should be determined for the future flux calculation. \(Q\) is approximated by a polynomial. Using this polynomial to approximate the value of \(Q\) at the left face fo the cell \(i\), \(Q_{i-\frac{1}{2}}\), which is the right side of the face at the face \(i - \frac{1}{2}\). It is straight forward to approximate the the value...
of $Q$ at the right face fo the cell $i$, $Q_{i+\frac{1}{2}}^l$, which is the left side of the face at the face $i+\frac{1}{2}$. In the same method, the left and right values at each cells will be defined.

The simplest reconstruction is the first order reconstruction. In this method, the conservative vector in each cell is same as value at cell center

$$Q_i(x) = Q_i$$ (3.78)

Therefore, the face values of cell $i$ are:

$$Q_{i-\frac{1}{2}}^r = Q_{i+\frac{3}{2}} = Q_i$$ (3.79)

This method is numerically diffusive and not suitable for the simulations in this dissertation. The third order accurate Modified Upwind Scheme for Conservative Laws (MUSCL) is used for all the simulation cases. The MUSCL reconstruction method employs the cell average values of $Q_{i-1}$, $Q_i$ and $Q_{i+1}$ to approximate $Q$ at cell $i$. We define a primitive function $I(x)$

$$I(x) = \int_{x_{i-\frac{3}{2}}}^{x} Q dx$$ (3.80)

where $x_{i-\frac{3}{2}} \leq x \leq x_{i+\frac{3}{2}}$. The distance between right face and left face of cell $i$ is defined as $\Delta x_i = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$ and it can change for non-uniform grid. From the definition of $I(x)$, $I(x)$ can be used at cells $i-1$, $i$ and $i+1$. Thus,

$$I\left(x_{i-\frac{3}{2}}\right) = 0$$ (3.81)

$$I\left(x_{i-\frac{1}{2}}\right) = \Delta x_{i-1} Q_{i-1}$$ (3.82)

$$I\left(x_{i+\frac{1}{2}}\right) = \Delta x_{i-1} Q_{i-1} + \Delta x_i Q_i$$ (3.83)

$$I\left(x_{i+\frac{3}{2}}\right) = \Delta x_{i-1} Q_{i-1} + \Delta x_i Q_i + \Delta x_{i+1} Q_{i+1}$$ (3.84)

There is a unique third order polynomial $P(x)$ to estimate $I(x)$ at four faces $x_{i-\frac{3}{2}}, x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}},$ and $i + \frac{3}{2}$. This polynomial is derived by using Newton’s formula

$$P(x) = a_0 + a_1 \left(x - x_{i-\frac{3}{2}}\right) + a_2 \left(x - x_{i-\frac{3}{2}}\right) \left(x - x_{i-\frac{1}{2}}\right)$$ (3.85)

$$= a_3 \left(x - x_{i-\frac{3}{2}}\right) \left(x - x_{i-\frac{1}{2}}\right) \left(x - x_{i+\frac{1}{2}}\right)$$ (3.86)
where

\[ a_0 = I\left[x_{i-\frac{3}{2}}\right] \] (3.87)
\[ a_1 = I\left[x_{i-\frac{3}{2}}, x_{i-\frac{1}{2}}\right] \] (3.88)
\[ a_2 = I\left[x_{i-\frac{3}{2}}, x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right] \] (3.89)
\[ a_3 = I\left[x_{i-\frac{3}{2}}, x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}, x_{i+\frac{3}{2}}\right] \] (3.90)

where

\[ I\left[x_{i-\frac{3}{2}}\right] = I\left(x_{i-\frac{3}{2}}\right) \] (3.91)
\[ I\left[x_{i-\frac{3}{2}}, x_{i-\frac{1}{2}}\right] = \frac{I\left[x_{i-\frac{3}{2}}\right] - I\left[x_{i-\frac{1}{2}}\right]}{x_{i-\frac{1}{2}} - x_{i-\frac{3}{2}}} \] (3.92)
\[ I\left[x_{i-\frac{3}{2}}, x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right] = \frac{I\left[x_{i-\frac{3}{2}}, x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right] - I\left[x_{i-\frac{3}{2}}, x_{i-\frac{1}{2}}\right]}{x_{i+\frac{1}{2}} - x_{i-\frac{3}{2}}} \] (3.93)
\[ I\left[x_{i-\frac{3}{2}}, x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}, x_{i+\frac{3}{2}}\right] = \frac{I\left[x_{i-\frac{3}{2}}, x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}, x_{i+\frac{3}{2}}\right] - I\left[x_{i-\frac{3}{2}}, x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right]}{x_{i+\frac{3}{2}} - x_{i-\frac{3}{2}}} \] (3.94)

To estimate \( Q \) at different locations, the reconstruction function \( Q(x) \) is defined as

\[ Q_i(x) = \frac{dP}{dx} \text{ for } x_{i-\frac{1}{2}} \leq x \leq x_{i+\frac{1}{2}} \] (3.95)

Therefore,

\[ Q_i(x) = a_1 + a_2 \left[ (x - x_{i-\frac{1}{2}}) + (x - x_{i-\frac{3}{2}}) \right] + a_3 \left[ (x - x_{i-\frac{1}{2}})(x - x_{i+\frac{1}{2}}) + (x - x_{i-\frac{3}{2}})(x - x_{i+\frac{3}{2}}) + (x - x_{i-\frac{3}{2}})(x - x_{i-\frac{1}{2}}) \right] \] (3.96)

Combining equations 3.86, 3.90, and 3.94, \( a_1, a_2 \) and \( a_3 \) for reconstruction function are

\[ a_1 = Q_{i-1} \] (3.99)
\[ a_2 = (\Delta x_i + \Delta x_{i-1})^{-1} \Delta Q_{i-\frac{3}{2}} \] (3.100)
\[ a_3 = [\Delta x_{i+1} + \Delta x_i + \Delta x_{i-1}]^{-1} \left( \frac{\Delta Q_{i+\frac{1}{2}}}{\Delta x_{i+1} + \Delta x_i} - \frac{\Delta Q_{i-\frac{1}{2}}}{\Delta x_i + \Delta x_{i-1}} \right) \] (3.101)
Using eqn (3.98), the left reconstruction to the face of cell \(i\) is the left side of face \(i + \frac{1}{2}\)

\[
Q_{i+\frac{1}{2}}^l = Q_i + \Delta Q_{i+\frac{1}{2}}^l \frac{(\Delta x_i + \Delta x_{i-1}) \Delta x_i}{(\Delta x_{i+1} + \Delta x_i)(\Delta x_{i+1} + \Delta x_i + \Delta x_{i-1})} \\
+ \Delta Q_{i-\frac{1}{2}}^l \frac{\Delta x_i}{(\Delta x_{i+1} + \Delta x_{i-1})(\Delta x_{i+1} + \Delta x_i + \Delta x_{i-1})} \\
Q_{i-\frac{1}{2}}^r = Q_i - \Delta Q_{i+\frac{1}{2}}^r \frac{(\Delta x_i + \Delta x_{i-1}) \Delta x_i}{(\Delta x_{i+1} + \Delta x_i)(\Delta x_{i+1} + \Delta x_i + \Delta x_{i-1})} \\
- \Delta Q_{i-\frac{1}{2}}^r \frac{\Delta x_i}{(\Delta x_{i+1} + \Delta x_{i-1})(\Delta x_{i+1} + \Delta x_i + \Delta x_{i-1})}
\]  

(3.102)  

(3.103)  

(3.104)  

(3.105)

These equations could be rewritten as shown below

\[
Q_{i+\frac{1}{2}}^l = Q_i + \Delta Q_{i+\frac{1}{2}}^l \kappa_{i+\frac{1}{2}}^l + \Delta Q_{i-\frac{1}{2}}^l \kappa_{i-\frac{1}{2}}^l \\
Q_{i-\frac{1}{2}}^r = Q_i - \Delta Q_{i+\frac{1}{2}}^r \kappa_{i+\frac{1}{2}}^r - \Delta Q_{i-\frac{1}{2}}^r \kappa_{i-\frac{1}{2}}^r
\]  

(3.106)  

(3.107)

where

\[
\kappa_{i+\frac{1}{2}}^l = \frac{(\Delta x_i + \Delta x_{i-1}) \Delta x_i}{(\Delta x_{i+1} + \Delta x_i)(\Delta x_{i+1} + \Delta x_i + \Delta x_{i-1})} \\
\kappa_{i-\frac{1}{2}}^l = \frac{\Delta x_i}{(\Delta x_{i+1} + \Delta x_{i-1})(\Delta x_{i+1} + \Delta x_i + \Delta x_{i-1})} \\
\kappa_{i+\frac{1}{2}}^r = \frac{(\Delta x_i + \Delta x_{i-1}) \Delta x_i}{(\Delta x_{i+1} + \Delta x_i)(\Delta x_{i+1} + \Delta x_i + \Delta x_{i-1})} \\
\kappa_{i-\frac{1}{2}}^r = \frac{\Delta x_i}{(\Delta x_{i+1} + \Delta x_{i-1})(\Delta x_{i+1} + \Delta x_i + \Delta x_{i-1})}
\]  

(3.108)  

(3.109)  

(3.110)  

(3.111)

\textit{GASPEX} allows the user to employ characteristic-based (upwind) flux functions for computing the flux, and these functions require two fluid-dynamic states at each cell face – the so-called left and right states. The accuracy of reconstructing the primitive variable field at the cell faces determines the spatial accuracy of the solution [53]. Considering using equations 3.107 and 3.111 on an uniform structured grid, a one-parameter family of interpolated values for the left state at the \(i + 1/2\) face and right state at the \(i - 1/2\) face can be represented as:

\[
Q_{i+1/2}^l = Q_i + \frac{\phi}{4}[(1 - \kappa) \nabla Q_i + (1 + \kappa) \Delta Q_i] \\
Q_{i-1/2}^r = Q_i - \frac{\phi}{4}[(1 + \kappa) \nabla Q_i + (1 - \kappa) \Delta Q_i]
\]  

(3.112)

where

\[
\Delta Q_i = Q_{i+1} - Q_i \\
\nabla Q_i = Q_i - Q_{i-1}
\]
and the spatial accuracy of the reconstruction is depends on the value for $\kappa$.

This method works well for interior cells and ghost-cell boundaries. However, the inviscid flux along a solid surface does not require a reconstruction because the primitive variables at the boundary face are known from the boundary condition. The flux is evaluated with the data provided at the wall. For the first interior face, the MUSCL formulation (i.e., eqn (3.112)) is altered to account for the position in space of the boundary data. For example, if a solid surface exists at an $i0$ boundary, the backward gradient is doubled (i.e., $\nabla Q \rightarrow 2\nabla Q = 2(Q_2 - Q_1)$) to account for the closer spacing between data points. A similar correction is applied for the forward gradient for an $idim$ solid wall.

In the GUI of GASPex, a first-order reconstruction (i.e., $\phi = 0$) is assumed if $\kappa$ is outside the range of $\kappa \in [-1, +1]$ . If the user inputs a high-order value of $\kappa$ in the marching direction, then GASPex assumes $\kappa = -1$. To assist the user, the value of $\kappa$ is set according to the spatial accuracy selected in the Inviscid tab of the GUI. For global flow fields, the common choices for $\kappa$ are:

- For computations in proposal, third-order upwind
  \[
  \kappa = -1 - \text{Second-order, fully upwind scheme. The linear reconstruction’s slope equals the fully upwind gradient, } q_i - q_{i-1}.
  \]

- Second-order, Fromm’s scheme. The linear reconstruction’s slope equals the symmetric gradient, $q_{i+1} - q_{i-1}$.

- Third-order, quadratic reconstruction which conserves the cell average of all three cells in the stencil: $q_{i-1}; q_i; q_{i+1}$.

- Central differencing. The linear reconstruction’s slope equals the downwind gradient, $q_{i+1} - q_i$.

biased, quadratic reconstruction ($\kappa = 1/3$) has been utilized.

### 3.6 Limiters

The reconstructions in eqn (3.112) without limiter may lead to numerical instability and oscillations in shock and other large gradient regions. The limiting process is needed to restrict the constructed primitive variable within the limits of the adjacent cell averages [50]. For example, if $Q_{i+1} > Q_i$, then the interface value, $Q_{i+1/2}$, should be within the
two adjacent limits (i.e., \( Q_i < Q_{i+1/2} < Q_{i+1} \)). Using a linear reconstruction on a uniform mesh, we can write the interface primitive variables as:

\[
Q_{i+1/2}^l = Q_i + \frac{1}{2} \left( \frac{\partial Q}{\partial x} \right) \Delta x \equiv Q_i + \frac{1}{2} \delta Q
\]

\[
Q_{i+1/2}^r = Q_i - \frac{1}{2} \left( \frac{\partial Q}{\partial x} \right) \Delta x \equiv Q_i - \frac{1}{2} \delta Q
\]

Comparing this Taylor series with the expressions given in eqn (3.112), we can identify \( \delta q \) as:

\[
\delta Q = \frac{1}{2} \left[ (1 - \kappa) \nabla Q_i + (1 + \kappa) \Delta Q_i \right]
\]

For a set of monotonically increasing primitive variables, the bounds of the forward and backward gradients are determined by limiting the interpolated cell-face primitive variables by \( Q_{i-1} \) and \( Q_{i+1} \). The adjacent cell averages are not exceeded as long as:

\[
Q_i - \frac{\delta Q}{2} \geq Q_{i-1} \text{ and } Q_i + \frac{\delta Q}{2} \leq Q_{i+1}
\]

We see that if the high-order gradient, \( \delta Q \), exceeds either \( 2\Delta Q_i \) or \( 2\nabla Q_i \), than the magnitude of the gradient should be reduced to fit within these extremes. We can reduce the gradient using a multiplicative filter function as:

\[
(\delta Q)_{limited} = R(\theta) \delta Q
\]

where \( \theta \equiv \Delta Q_i / \nabla Q_i \) is the ratio of the forward to the backward gradients. By equating the limits of the gradient magnitude to the filtered reconstruction, we obtain:

\[
\min(2\Delta Q_i, 2\nabla Q_i) = R(\theta) \left\{ \frac{1}{2} \left[ (1 - \kappa) \nabla Q_i + (1 + \kappa) \Delta Q_i \right] \right\}
\]

(3.113)

We can then see the filter is

\[
R(\theta) = \min \left[ \frac{4}{(1 - \kappa) + (1 + \kappa)\theta}, \frac{4\theta}{(1 - \kappa) + (1 + \kappa)\theta} \right]
\]

The choice of \( R(\theta) = 1 \) must be available to exactly reconstruct linear data (i.e., when \( \Delta Q_i = \nabla Q_i \)). In GASPex limiting is applied in two different ways: limiting of the primitive variables and limiting performed in the marching direction. The Limiting parameter in the GUI controls the limiting performed in each of the coordinate directions. The limiting
options can be found in the Inviscid tab of the GUI (under Physical Models). Primitive-variable limiting means that the particular limiter model (e.g., MIN-MOD) is applied to the forward and backward gradients of the primitive variables. These limited gradients are then applied in eqn (3.112) to obtain the reconstructed values of the left and right states. The exact form of the limited equation depends on the model selected. In this proposal, Van Albada’s and Min-Mod limiters are used in simulations.

3.6.1 Van Albada’s Limiter

Van Albada’s limiter [55] was designed in the context of Fromm’s scheme (i.e., $\kappa = 0.0$) so that the high-order corrections in eqn (3.112) would tend to the average of the gradients in smooth regions and to the smaller gradient otherwise. Setting $\kappa = 0$, the Van Albada’s filtering function in eqn (3.113) is:

$$R(\theta) = \frac{2\theta}{\theta^2 + 1}, \ \theta > 0$$

3.6.2 The Minimum Modulus (Min-Mod) Limiter

The min-mod function chooses the smaller of the two gradients (forward and backward) by magnitude if they have the same sign and zero otherwise. The function can be written as:

$$\text{minmod}(x, y) = \begin{cases} x & |x| < |y| \text{ and } xy > 0 \\ y & |y| < |x| \text{ and } xy > 0 \\ 0 & xy < 0 \end{cases}$$ (3.114)

3.7 Viscous flux

To calculate the viscous flux, we must approximate derivatives at cell face and the second order central differencing is used at here. For all interior cell face [50],

$$\left( \frac{\partial \phi}{\partial x_i} \right)_{j+\frac{1}{2}} = (\phi_{j+1} - \phi_j) \frac{A_{j+\frac{1}{2}}}{Vol_{j+\frac{1}{2}}} \hat{n}_{x_i}$$ (3.115)

where $\phi$ represents arbitrary scalar variable, $x_i$ is one of the three Cartesian directions and $j$ is one of three cell index. $A_{j+\frac{1}{2}}$ is the face area and $Vol_{j+\frac{1}{2}}$ is an average of the two adjacent
cell volumes. \( \hat{n}_{x_i} \) is the unit normal of the face in one of the three Cartesian directions.

For the boundary face, the second order wall gradient is

\[
\left( \frac{\partial \phi}{\partial x_i} \right)_{wall} = -\frac{\phi_3 + 7\phi_2 - 6\phi_1}{2} \frac{A}{Vol} \hat{n}_{x_i}
\]

(3.116)

where \( \phi_2 \) and \( \phi_3 \) is the first and second interior cells value, \( \phi_1 \) is the wall value (see Fig. 3.2), \( A \) is the boundary face area and \( Vol \) is the first interior cell volume.

### 3.8 Time Integration Methods

#### 3.8.1 Steady State Simulation

The computation for Run 1 is steady state simulation. In GASPEX, the steady state simulation is performed using an Euler Implicit algorithm where a constant time step is used to produce a pseudo first-order solution. The Euler implicit method takes a non-linear PDE and turns it into a linear system that can be solved by one of the algorithms in the time integration. In Run 1, the solver scheme used is Gauss-Seidel which is an iterative technique for linear systems. GASPEX implements a symmetric Gauss-Seidel solver which carries out a forward and a backward sweep on every iteration. The number of iterations per step is set to 10. The relative and absolute convergence criteria of \( 10^{-6} \) and \( 10^{-12} \) respectively in Run 1. The time step set to constant \( Dt \) because varying cell spacing inside grid. \( Dt \) was chosen to be

\[
Dt = \frac{t_c}{10000}
\]

(3.117)

where characteristic time \( t_c = \frac{L}{u_{\infty}} \) and \( L \) is the length of total domain.

#### 3.8.2 Implicit Dual Time Scheme

Run 2 uses the second order Implicit Dual Time scheme which is an implicit formulation attaining second order time accuracy while allowing implicit treatment of the fluxes and source terms. This method has a outer loop using the real time of computation \( (t) \) and a inner loop using a pseudo time \( (\tau) \). Some implicit methods which cannot maintain time accuracy can be utilized in the inner loop because time accuracy is defined by real time in
the outer loop [50]. The implicit governing equations with a pseudo-time derivative become:

\[
\frac{\partial}{\partial \tau} \iiint QdV = - \left( \frac{\partial}{\partial \tau} \iiint_{V(t)} Qdv + \iiint_{S(t)} \left( \vec{F} - \vec{F}_v \right) \cdot \hat{n} dS \right)^{m+1} \tag{3.118}
\]

where \( m \) represents a discrete solution in pseudo-time \( \tau \). In each real time step, the implicit equations solved be inner iterations and set converged solution of the inner iteration as the result of the next real time level \( n + 1 \).

In Run 2 and 3, time step in outer loop is set to \( 10^{-7} \) s and the number of inner iterations per step is set to 10. The relative and absolute convergence criteria of \( 10^{-6} \) and \( 10^{-12} \) respectively. In the inner iteration, time step is calculated on the basis of the CFL:

\[
\Delta t = \frac{\lambda \Delta L}{c} \tag{3.119}
\]

where \( \lambda \) is the Courant number, \( \Delta L \) is the characteristic length of the cell and \( c \) is the characteristic velocity. A fixed \( CFL = 1 \) and automated time step limiting is used in Run 2 and 3. The characteristic velocity is calculated on the local cell quantities.

### 3.9 Boundary Condition

In the numerical simulations, properly boundary conditions are necessary. In GASPex, boundary conditions apply in different ways. One method is directly applying primitive variables value at the boundary as shown in the right side of Fig. 3.2. The primitive variables are calculated from the flux at the boundary. Another method is assigning primitive values at two imaginary ghost cells beyond the physical domain to split flux at the boundary face as shown in the left side of Fig. 3.2.
The computational domain and boundary conditions can be found below:

Boundary AB is set to Axisymmetric Lines. The flux at the boundary with axisymmetric boundary is zero because the surface area is zero. As for flow quantities, dependent variables around the axis are equal but the signs of two velocity components are reversed and along the axis would not change.

Face BC is set to the freestream boundary condition. As for the case in this dissertation, the inflow freestream Mach number is above sonic which means all the eigenvalues are positive and all flow information propagates downstream. Therefore, the primitive variables
at the boundary can be fixed to the values of the freestream. In GASPex, the "Fixed at Q" is designed for this kind of situation and this boundary condition applied using ghost cells. These primitive variables at the ghost cell are fixed at the freestream values which determined by user defined static temperature, static pressure and the Mach number in the Q Spec tab located at the Physical Models frame as shown in Fig. 3.4.

![Figure 3.4: Q Spec Input](image)

Face CD is the outflow boundary and the "Extrapolation" condition is used at here. Originally, the extrapolation should be applied for hypersonic or supersonic flow where all the characteristic lines of the flow move exit the computational domain. In this dissertation’s case, the extrapolation can be selected because most of region at the exiting is supersonic and only a small subsonic region of fully developed boundary layer existence which means there is no rapid change of flow gradient in the normal direction to the outflow boundary. In GASPex, the extrapolation condition is applied by extrapolating the primitive variables from the interior cells to the ghost cells. The extrapolation can be either first or second order accurate by using different number of ghost cells and the first order extrapolation was used after considering the computations performed.

Face DA is set to "No Slip Isothermal Wall". In GASPex, the no slip isothermal wall boundary is implemented by directly assigning the user-specified primitive variable at the boundary. The velocity components are set to zero for no slip conditions. The boundary temperature is set to the user defined wall temperature, the pressure is extrapolated from the interior and the density is calculated using the equation of the state, $p = \rho RT$. 
Two side faces are set to "Positive/Negative Axisymmetric Walls". When these conditions implement, the velocity vector of the ghost cell at the boundary cell is generated through the interior velocity rotated about the singular axis.

In summary, the boundary conditions are defined in the Tables 3.1 to 3.5. For reference, as shown in Fig. 3.2, a subscript 0 refers to the ghost cell beyond the interior cells if applied boundary condition through ghost cell as shown in the left side of figure or refers to the solid boundary if directly assign primitive variables at the boundary as shown in the right side of Fig. 3.2, a subscript 1 refers to the first interior cell and subscript 2 refers to the second interior cell from the boundary.

Table 3.1: Boundary conditions: Axisymmetric Line

<table>
<thead>
<tr>
<th></th>
<th>((\rho_i)_1 = (\rho_i)_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass fraction density</td>
<td>((\rho_i)_1 = (\rho_i)_2)</td>
</tr>
<tr>
<td>Density</td>
<td>(\rho_1 = \rho_2)</td>
</tr>
<tr>
<td>Velocity components</td>
<td>(u_1 = u_2, ; v_1 = -v_2, ; w_1 = -w_2)</td>
</tr>
<tr>
<td>Pressure</td>
<td>(p_1 = p_2)</td>
</tr>
<tr>
<td>Temperature</td>
<td>(T_1 = T_2)</td>
</tr>
</tbody>
</table>

Table 3.2: Boundary conditions: Fixed at Q

<table>
<thead>
<tr>
<th></th>
<th>((\rho_i)_0 = (\rho_i)<em>1 = (\rho_i)</em>\infty)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass fraction density</td>
<td>((\rho_i)_0 = (\rho_i)<em>1 = (\rho_i)</em>\infty)</td>
</tr>
<tr>
<td>Density</td>
<td>(\rho_0 = \frac{p_0}{RT_0} = \frac{p_1}{RT_1} = \rho_1 = \frac{p_\infty}{RT_\infty} = \rho_\infty)</td>
</tr>
<tr>
<td>Velocity components</td>
<td>(u_0 = u_1 = u_\infty, ; v_0 = v_1 = v_\infty, ; w_0 = w_1 = w_\infty)</td>
</tr>
<tr>
<td>Pressure</td>
<td>(p_0 = p_1 = p_\infty)</td>
</tr>
<tr>
<td>Temperature</td>
<td>(T_0 = T_1 = T_\infty)</td>
</tr>
</tbody>
</table>
Table 3.3: Boundary conditions: extrapolation

<table>
<thead>
<tr>
<th>Mass fraction density</th>
<th>((\rho_i)_0 = (\rho_i)_1 = (\rho_i)_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>(\rho_0 = \frac{\rho_0}{RT_0} = \frac{\rho_1}{RT_1} = \rho_1 = \frac{\rho_2}{RT_2} = \rho_2)</td>
</tr>
<tr>
<td>Velocity components</td>
<td>(u_0 = u_1 = u_2, v_0 = v_1 = v_2, w_0 = w_1 = w_2)</td>
</tr>
<tr>
<td>Pressure</td>
<td>(p_0 = p_1 = p_2)</td>
</tr>
<tr>
<td>Temperature</td>
<td>(T_0 = T_1 = T_2)</td>
</tr>
</tbody>
</table>

Table 3.4: Boundary conditions: isothermal, no-slip wall

<table>
<thead>
<tr>
<th>Mass fraction density</th>
<th>((\rho_i)_1 = \left(\frac{\rho_i}{\rho}\right)_2 \rho_1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>(\rho_1 = \frac{\rho_1}{RT_1})</td>
</tr>
<tr>
<td>Velocity components</td>
<td>(u_1 = 0, v_1 = 0, \frac{\partial w_1}{\partial z} = 0)</td>
</tr>
<tr>
<td>Pressure</td>
<td>(p_1 = p_2)</td>
</tr>
<tr>
<td>Temperature</td>
<td>(T_1 = 297 K)</td>
</tr>
</tbody>
</table>

Table 3.5: Boundary conditions: Positive/Negative Axisymmetric Walls

<table>
<thead>
<tr>
<th>Mass fraction density</th>
<th>((\rho_i)_1 = (\rho_i)_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>(\rho_1 = \rho_2)</td>
</tr>
<tr>
<td>Velocity components</td>
<td>(u_1 = u_2, v_1 = v_2 \cos(2.25^\circ) - w_2 \sin(2.25^\circ), w_1 = v_2 \sin(2.25^\circ) + w_2 \cos(2.25^\circ))</td>
</tr>
<tr>
<td>Pressure</td>
<td>(p_1 = p_2)</td>
</tr>
<tr>
<td>Temperature</td>
<td>(T_1 = T_2)</td>
</tr>
</tbody>
</table>

3.10 Initial Condition

For steady state simulation Run 1, the initial condition for the coarsest grid (0.56M grid in Table 3.6) is set to the freestream conditions 1 mentioned in Table 2.1. Steady state simulation result from the coarsest grid will be used as the initial conditions for the finer grid through interpolating the coarsest grid result to the next sequence level grid.

As for time accurate simulations Run 2 and Run 3, the freestream conditions 1 is used for initial conditions for all the grids.
3.11 Grid Generation

The grid is generated in MATLAB R2020b in PLOT3D format. PLOT3D is a widely used file format for grid and result storage [56]. The wall-normal span of the grid at the end of first cone to set up to above 90 mm, allowing for the bow shock and separation zone to be fully contained within the grid [1]. The grid is clustered in the high gradient region (wall shown in Fig. 3.5 and nosetip shown in Fig. 3.6).

Figure 3.5: Grid at cone/flare junction.
Figure 3.6: Grid at nosetip

The grid details are given in Table 3.6.

<table>
<thead>
<tr>
<th>Grid</th>
<th>idim</th>
<th>jdim</th>
<th>$\Delta x$ ($\mu$m)</th>
<th>$\Delta y$ ($\mu$m)</th>
<th>Number of Cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sequence 1</td>
<td>1126</td>
<td>501</td>
<td>171.5</td>
<td>3.0</td>
<td>564,126</td>
</tr>
<tr>
<td>Sequence 2</td>
<td>2251</td>
<td>501</td>
<td>343</td>
<td>3.0</td>
<td>1,127,751</td>
</tr>
</tbody>
</table>

Legend:

$idim$ no. of cells in the streamwise direction

$jdim$ no. of cells in the direction normal to wall

$\Delta x$ average spacing between grid cells in streamwise direction

$\Delta y$ minimum spacing between grid cells in normal direction from wall
3.12 Zonal Decomposition

GASPex can divide a zone into several partitions where each zone is then sent to different processors to run parallel. It will reduce CPU load, memory usage for each processor and improve entire computational efficiency. All of the computations in this dissertation are performed on the Rutgers School of Engineering HPC cluster where the computational zone is decomposed into 144 parts in GASpex.
Chapter 4

Results

In this dissertation, the heat transfer data collected from the numerical simulations is compared with the experimental result. The non-dimensional heat flux Stanton number $St$ is the heat transfer data used in this section. The equation for Stanton number is shown below:

$$St = \frac{\dot{q}}{\rho_{\infty} u_{\infty} c_p (T_0 - T_{wall})}$$

(4.1)

where $\dot{q}$, $\rho_{\infty}$, $u_{\infty}$, $c_p$, $T_0$, and $T_{wall}$ are the heat flux, freestream density, freestream velocity, specific heat capacity, stagnation temperature, and wall temperature.

In the experiment, the separation point can be identified at the location of Stanton number slope abruptly decreases for a laminar boundary layer [1]. The separation point is numerically defined as the location where

$$\left| \frac{dSt}{d(x/L)} \right| > 600\%$$

(4.2)
4.1 Convergence Study

Figure 4.1: Stanton number for Run 1 in 0.56M cells

The steady state simulation Run 1 was performed on 0.56M grid and 1.12M grid. Fig. 4.1 above is the heat transfer data from Run 1 in 0.56M grid, the $x$ coordinate has been non-dimensionalized by the distance from the nosetip of the first cone to the cone/flare junction location, $L$ and $y$ coordinate is the Stanton number mention in eqn (4.1). The location change of separation point is less than 10% after 150000 steps in 0.56M grid.

Fig. 4.2 below is the heat transfer data from Run 1 in 1.12M. Steady state simulation results from 0.56M cells grid after 250000 steps were used as initial conditions for simulations in 1.12M cells grid and the separation point was unchanged from 50000 steps to 250000 steps in 1.12M grid. Therefore, steady state simulation Run 1’s results were converged to steady state after 250000 steps for both 0.56M and 1.12M grid.
The time accurate simulation Run 2 and Run 3 were performed on same grids. Fig. 4.3, Fig. 4.4, Fig. 4.5 and Fig. 4.6 are the Stanton number profile from Run 2 and Run 3. In these figures, the location change of separation points are close after 0.02 s which is 35.4 dimensionless times. One dimensionless time is the time required for the freestream to pass the first cone. The time accurate result used in the later section were collected at 0.05 s which is equal to 88.5 dimensionless time. Thus, time accurate results used in the later section collected from Run 2 and Run 3 were converged to steady state at 0.05s.
Figure 4.3: Stanton number for Run 2 in 0.56M cells

Figure 4.4: Stanton number for Run 2 in 1.12M cells
Figure 4.5: Stanton number for Run 3 in 0.56M cells

Figure 4.6: Stanton number for Run 3 in 1.12M cells
4.2 Flow Patterns

The flow pattern presented here are based on the numerical simulation results. Fig. 4.7 is the entire flowfield structure for Run 1 after 30000 steps in 0.56M grid. Run 1 is the steady state simulations of test flow 1 over double cone with 10.2 mm radius nose and 37 degree flare.

First, we consider the flows over blunt nose. The static pressure $p$ ahead of the blunt nose abruptly increases because of the bow shock wave generated by the bluntness. As shown in the Fig. 4.8 below, the bow shock can be found at the top of the image.
Comparison of numerical results and analytical predictions is possible. The analytical predictions of oblique bow shock wave angle could be obtained from a Taylor-Maccoll solution. The equation of this method is shown in eqn (4.3) [3], which is an ordinary differential equation. Using the freestream Mach number and inviscid flow shock angle, we can calculate numerical solution of this ordinary differential equation.

\[
\frac{\gamma - 1}{2} \left[ V_{\text{max}}^2 - V_r^2 - \left( \frac{dV_r}{d\theta} \right)^2 \right] \left[ 2V_r + \frac{dV_r}{d\theta} \cot\theta + \frac{d^2V_r}{d\theta^2} \right] \left[ 2V_r + \frac{dV_r}{d\theta} \cot\theta + \frac{d^2V_r}{d\theta^2} \right] = 0
\]

where \(\gamma\) is specific heat ratio, \(V_{\text{max}}\) is maximum theoretical velocity, \(V_r\) is radial component of velocity and \(\theta\) is shock wave angle.

Using Taylor-Maccoll theory can predict a bow shock of 11.82° to the freestream at Mach number of 6.1 under the assumption of a 7° half-angle cone incorporating a sharp tips and has an infinite length [3].

The bow shock angle from numerical simulations is 13.1° which is not exactly same with predicted bow shock angle. The reason is that the prediction through Taylor-Maccoll is based on sharp cone tip. As for a cone with the bluntness tip, the oblique shock will be influenced by the normal shock at the upstream of the nose which would make angle not
same as predication.

At the bluntness nose, the shock detachment distance $\delta$ can be calculated from hypersonic shock wave shape correlations, which is based on the experimental data. The equation for sphere-cone is shown below [57]:

$$\frac{\delta}{R} = 0.143 \exp \left( \frac{3.24}{M_{\infty}^2} \right)$$

(4.4)

where $R$ is the radius of the nose.

From eqn (4.4), the detachment distance is 1.59 mm and the detachment distance from the numerical result is 1.55 mm. The computational result shows agreement with predication for the shock detachment distance.

After the bow shock wave, a thin sublayer can be defined by gas passing through the bow shock at upstream of the nose. This thin sublayer is called high-entropy layer (HEL). Then, the thickness of boundary layer is increased along the first cone.

Figure 4.9: Mach numbers around flare of Steady State Simulation after 30000 steps in 0.56M grid.

As for the cone/flare junction region shown in Fig. 4.9, an adverse pressure gradient is generated by the flare. The near wall gas inside the boundary layer is blocked by the high adverse pressure region near the flare and causes separation of the boundary layer with a separation shock. Gas at the boundary of the separation layer is able to move into the high
pressure region after acquires sufficient momentum from the external flow and generates a mixing layer. Inside the separation zone, part of the blocked high-entropy layer circulates together with the boundary layer and forms recirculation in separation region. At the end of the separation zone, the boundary layer reattaches the flare and extreme pressure rise and heat flux increases are predictable.

The separation region continues to enlarge until 250000 steps and the Mach number contours for steady state case Run 1 at 250000 steps are shown in Fig. 4.10. Comparing with the result at 30000 steps, the starting point of the separation zone is almost reaching the cone tip and the reattachment point is located at the end of the flare.

![Mach number contours](image)

Figure 4.10: Mach numbers of Steady State Simulation after 250000 steps in 0.56M grid.

To confirm the result from steady state simulation, Run 2 and Run 3 were performed to achieve steady state as mentioned in the experiments through time-accurate simulations. In Run 2 and Run 3, the same grids were imported into GASPex and performed simulations using Roe’s method & Albada limiter and Van Leer’s method & min mod limiter with implicit dual time stepping methods. The Mach number contours at the 0.05 s from Run 2 and Run 3 are shown in Fig. 4.11 and Fig. 4.12. The flow pattern from the time-accurate simulations is close to the result from 250000 steps in Run 1.
Figure 4.11: Mach numbers of Time Accurate Simulation with Roe’s method after 0.05 s in 0.56M grid.

Figure 4.12: Mach numbers of Time Accurate Simulation with Van Leer method after 0.05 s in 0.56M grid.
4.3 Comparison with Experiment

4.3.1 Steady State Simulations

Fig. 4.13 above shows the Stanton number for blunt cone alone without flare. The grids for blunt cone in Fig. 4.13 are same with corresponding section in 0.56M and 1.12M grid. The computation result of the blunt nose alone agrees closely with the experimental data at the upstream of interaction region. Therefore, simulation of the flow developing on the cone is validated.

The Stanton number profile for Run 1 in 0.56M grid from 50000 steps to 250000 steps is shown in Fig. 4.1. Detailed Stanton number profile around the separation point in 0.56M grid is shown in Fig. 4.14, the separation point locates at $x/L = 0.49$ in 50000 steps and the Stanton number at the upstream of the separation agrees well with experiment and within
the uncertain of experiment. The separation point continues move upstream through iteration steps increasing. Until 250000 steps, the separation point is steady at $x/L = 0.067$. As for the location of peak $St$ value, the peak $St$ at 250000 steps is at the downstream of the corresponding point in experiment. Fig. 4.2 showed Run 1’s result from 1.12M grid, the location of the separation point from 1.12M is unchanged during simulation and is same as corresponding point from 0.56M. The size of computed separation zone is significantly larger than the experiment.

![Stanton Number before $x/L < 0.4$ in Run 1](image)

**Figure 4.14:** Stanton Number before $x/L < 0.4$ in Run 1

### 4.3.2 Time Accurate Simulations

To confirm steady state result, time accurate simulation Run 2 were performed in same grid. Run 2’s inviscid flux algorithm (Van Leer method), reconstruction and limiter(min-mod) setups were the same as Run 1. Fig.4.15 shows the Stanton number collected from 0.56M
cells grid at 0.05s. The separation point is located at $x/L = 0.065$ in Van Leer method (Run 2).

Fig.4.16 showed Stanton number collected from 1.12M cells grid at 0.05 s in Run 2. The separation point is located at $x/L = 0.061$ for Van Leer method (Run 2).

Another time accurate case Run 3 used different inviscid flux (Roe’s method) and limiter (Van Albada) were performed in the same grid. As shown in the Fig.4.15 and Fig.4.16, the separation point is located at $x/L = 0.063$ in 0.56M grid and $x/L = 0.057$ in 1.12M grid in Run 3 at 0.05 s.

### 4.3.3 Discussion

Results above showed that steady state Run 1 and time accurate simulations Run 2 and 3 predicted essentially the same separation point. Thus, the separation region in the simulations performed are insensitive to the inviscid flux and limiter chosen but the predicted separation result data differ substantially from the experiment. This suggests that the experimental data collected may not correspond to steady state.
Figure 4.15: Time Accurate simulation in 0.56M cells after 0.05 s
Figure 4.16: Time Accurate simulation in 1.12M cells after 0.05 s

(a) Stanton Number for entire model

(b) Stanton Number before $x/L < 0.4$
Chapter 5

Conclusion

Computational simulations of hypersonic laminar flow over a blunt cone flare has been performed using perfect gas laminar Naiver-Stokes equations in GASPeX. The steady state simulation result is close to time-accurate simulation and the influence from different combinations of inviscid flux methods and limiters is negligible. Heat transfer data at the upstream of SWBLI region agrees well with the experiment but the computed separation zone is significantly larger than the experiment, suggesting that the experimental data does not converge to steady state.
References


