

INVESTIGATION OF HIGH-RESOLUTION METHODS IN LARGE EDDY SIMULATION OF SUBSONIC AND SUPERSONIC WALL TURBULENT FLOWS

By

Ioannis William Kokkinakis

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Ioannis William Kokkinakis

Investigation of High-Resolution Methods in Large Eddy Simulation of Subsonic and Supersonic Wall Turbulent Flows

Ioannis William Kokkinakis

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Abstract

This thesis presents the motivation, objectives and reasoning behind the undertaken PhD to investigate the capability of compressible Implicit Large Eddy Simulation (ILES) in simulating wall-bounded inhomogeneous flows with particular interest in the near wall region and further presents the progress achieved to date. Investigation includes the assessment of current ILES methods to resolve inhomogeneous turbulence as well as compressible turbulent boundary layers and to improve on those models further.

A channel flow is an excellent problem to use to investigate the properties of a SGS model near a wall. The presence of a solid boundary tends to alter the behaviour of the turbulent flow in a number of ways that need to be modeled by the SGS model in order to correctly represent the flow near the wall and most importantly the boundary layer. The presence of the wall inhibits the growth of the small scales, alters the exchange mechanisms between the resolved and unresolved scales and finally gives rise in the SGS near wall region to important Reynolds-stress producing events.

A literature survey was carried out to identify other numerical investigations in simulating channel flow as well as data that could be used for validation purposes. The main parameters used to validate the level of resolution in simulating channel flow are identified and a number of tools are developed. The primary parameters extensively used to validate LES simulations of channel flow throughout the literature are mean flow velocity profiles, turbulent kinetic energy, dissipation and shear stress profiles, wall shear stress and friction velocities as well as energy spectra in the spanwise and streamwise homogeneous directions.

Compressible viscous ILES of inhomogeneous anisotropic turbulence in an incompressible channel flow at wall normal grid resolutions of 68, 96 and 128 cells are carried out with grid clustering applied to the wall normal direction. Initial results conducted in the compressible regime show that in order to obtain satisfactory results, medium and

fine grids are required whereas on coarser grids, some additional numerical method is required. Each reconstruction scheme introduces a numerical dissipation characteristic to itself that maybe regarded as a sort of turbulence model. Thus depending on the required dissipation, a suitable limiter can be chosen.

The investigation then moves on to supersonic turbulent flow incorporating shock-boundary layer interaction. Only the slope-limiters that prove to simulate the flow in the fully developed turbulent channel best are favoured and then also utilised in the subsequent compressible ramp simulations. The capabilities of modelling the shock boundary layer interaction, mean turbulent profiles and shockwave angle are investigated and compared against those obtained by DNS simulations. It is found that the grid at the inlet of the ramp plays a significant role, since it needs to be fine enough to maintain the turbulent inflow at an acceptable level before reaching the shock-boundary layer interaction zone. Further, very high-order numerical reconstructions were found to have difficulties in remaining stable in the high gradient regions of the flow when formulated in conservative form and therefore solutions were not possible to obtain. Nonetheless, lower order reconstruction methods run smoothly and the momentum profiles obtained, matched closely those obtained by DNS.

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Abbreviations

Acronyms

NSE	Navier Stokes Equations
PDE	Partial Differential Equations
CFD	Computational Fluid Dynamics
CPU	Computer Processor Unit
RANS	Reynolds Averaged Navier Stokes
URANS	Unsteady RANS
DNS	Direct Numerical Simulation
SGS	Sub Grid Scale
LES	Large Eddy Simulation
ILES	Implicit LES
MILES	monotonically Intergrated LES
FVM	Finite Volume Method
CV	Control Volume
AuxCV	Auxiliary CV
EoS	Equation of State
FVSM	Flux Vector Splitting Method
FDSM	Flux Difference Splitting Method
RK	Runge-Kutta
TVD	Total Variation Diminishing
MUSCL	Monotone Upstream-centred Schemes for Conservation Laws
VL	Van Leer
MC	Monotonized Central
ENO	Essentially Non-Oscillatory
WENO	Weighted Essentially Non-Oscillatory
CBS	Characteristics Based Scheme
HLL	Harten, Leer, Lax
HLLC	Harten, Leer, Lax Contact
LMNT	Low Mach Number Treatment
PIV	Particle Image Velocimetry

Greek Symbols

λ	kinematic viscosity
ϵ	dissipation rate
η	Kolmogorov length scale
u_η	Kolmogorov velocity scale
τ_η	Kolmogorov time scale
ψ	arbitrary quantity
δ	turbulent boundary layer thickness
α_{cc}	compression corner angle
ρ	density
$\bar{\bar{\tau}}$	shear stress tensor
μ	dynamic viscosity coefficient
ν	second viscosity coefficient
ϕ	slope limiter function
π	polynomial function
Π	weighted average polynomial function
α	speed of sound
β	forcing term
δ_{ij}	Kronecker symbol
τ_w	wall shear stress
ε	perturbation
Φ	local cell slope angle
$\vec{\alpha}$	arbitrary vector field
χ	scalar field

Latin Symbols

Re	Reynolds number
$\vec{n}$	unit normal vector
A	area
dA	elemental surface area
V	Volume
dV	elemental volume
$\vec{u}$	velocity vector
t	Real time
$\vec{f}$	body forces
p	pressure
E	total energy
e	internal energy
KE	kinetic energy
$\dot{q}$	heat flux
T	absolute static temperature
k	thermal conductivity coefficient
R	specific gas constant
Pr	Prandtl Number
S_u	Sutherland temperature
c_p	specific heat at constant pressure
c_v	specific heat at constant volume
γ	specific heat ratio
$\vec{F}_c$	convective flux
$\vec{F}_v$	viscous flux
$\vec{Q}$	source term
$\vec{W}$	vector of conservative variables
$\vee$	contravariant velocity
$\vec{B}$	body forces
$\vec{f}$	left running face diagonal
$\vec{g}$	right running face diagonal
$\vec{q}$	x running mid-volume vector
$\vec{r}$	y running mid-volume vector
$\vec{s}$	z running mid-volume vector

R	Residual
c	speed of characteristic
n	timestep number
m	RK stage number
s	wave speed
C	CFL number
r	slope
IS	smoothness indicators
Re_τ	friction Reynolds number
Re_m	bulk Reynolds number
M	Mach number
u^+	Velocity non-dimensionalised by friction velocity
u_τ	friction velocity
u_0	centreline velocity
Q	massflux
C_f	coefficient of friction

Introduction

1

Introduction

Fluid flow is everywhere. Our speech, our movements, the blood flow inside us, the sea, the atmosphere, all are governed by a set of mathematical equations. The most widely accepted in doing so well are the **Navier-Stokes Equations (NSE)**, named after Claude-Louis Navier and George Gabriel Stokes who the former derived the NSE in a paper in 1822 and the latter published in 1845 a derivation of the equations in a manner that is currently understood. However centuries old now, the solution of this set of equations has been troublesome ever since they were postulated for a number of reasons. For one, as already mentioned, it is a set of equations and not a single equation and therefore their solution requires a tedious process, that of solving a set of simultaneous equations. What is of greater significance though is that the terms involved are partial differentials which eventually lead to a set of non-linear **p**artial **d**ifferential **e**quations (PDE). For flows of any nature, laminar or turbulent, incompressible or compressible, subsonic or hypersonic, trying to solve these equations by pen and paper as was the norm when the NSE were developed and for a long time after, can be justly considered cumbersome.

Things started to change though with the invention of the transistor and its application to computers in the early 1960's. The speed and amount of computations the processors

were capable of, even at that early period far exceeded that of a human and it eventually enabled scientists to start solving the NSE computationally. Thus a new area of fluid dynamics was born, that of **computational fluid dynamics (CFD)**.

However, solving the NSE was still both a cumbersome and computationally demanding task even when utilising the computer, which at the time could be considered of having minor capabilities by today's standards and hence limited CFD in all areas, from the grid size to the numerical methods employed. Only flows with certain properties could be calculated (2-Dimensional Low Reynolds (Re) Flows) using various approximations such as incompressibility and non-viscous assumptions in order to simplify the NSE.

With time, the computational capabilities of the **computer processor unit (CPU)** increased following Moore's famous law which was stated back in 1965 and predicted the doubling of the transistors every couple of years. Ever since, it has been maintained and remarkably still holds true up to today. The development along with projections made for the near future of the available computer resources can be seen below in Figure 1.1.



FIGURE 1.1: Available processing speed power over time [1]

As computers became more powerful and an ever increasing number of people became involved in CFD research and development, an "explosion" in the number of new numerical methods and theories being devised occurred, which eventually helped CFD increase the range of flows it was capable of solving and consequently reached a point where higher Reynolds flows were trying to be modeled. The high Reynolds numbers though introduced an old classical problem in fluid dynamics, that of turbulence. The nonlinear part of the NSE, that is the convective term, is responsible for the generation of as is known today, turbulence. This is a region of the flow that always alters with time and

is dominated of what seems as an unorderly motion such as that seen in Figure 1.2. Even today there is no widely accepted theory on turbulence and that which exists corresponds to ideal cases that make various assumptions and approximations. Such a case is isotropic turbulence theory which assumes for example that the turbulent scales remain the same in the whole domain considered.



FIGURE 1.2: Turbulence in a streak of smoke [2]

Today, there exist mainly three methods that have been developed to deal with solving the NSE, differentiated by their approach in modelling turbulence. Those are **R**eynolds-**A**veraged-**N**avier-**S**tokes (RANS), **L**arge-**E**ddy-**S**imulation (LES) and **D**irect-**N**umerical-**S**imulation. A brief overview of these three methods will be given with regards to how they resolve turbulence and what each method's advantages and disadvantages are.

DNS tries to resolve all scales up to the Kolmogorov scale [5] for which estimates for the length, velocity and time-scales are given as functions of kinematic viscosity ν and dissipation rate ϵ by [6]

$$\eta \sim \left(\frac{\nu^3}{\epsilon} \right)^{1/4} \quad u_\eta \sim (\nu\epsilon)^{1/4} \quad \tau_\eta \sim \left(\frac{\nu}{\epsilon} \right)^{1/2}$$

It is the most straightforward approach to the solution of turbulent flows since the Navier-Stokes equations are discretised directly and solved numerically on grids fine enough to allow all turbulent scales of motion to be resolved. Thus with DNS one can obtain an accurate three-dimensional, time-dependent and modelling-free (no use of turbulence models) solution of the governing equations in which the only errors are those introduced by the numerical approximation. However, the use of highly accurate, high-order schemes to minimise numerical dispersion and dissipation errors as well as the fact that the meshes used require a number of points that can be shown to be proportional to the $9/4$ power of the Re number and a computational scale cost proportional to Re number cube limits the application of DNS to flows in simple geometries at low Re numbers, typically lower than 10^5 , and its application to engineering-type problems in the next decade seems unlikely. To enforce this, [7] showed that 10^{16} grid points and several thousand years on a 10^{12} Flop computer are required in order to simulate the flow over a Jumbo jet flying at cruise speed for one second of flight at a Re number of typically 10^8 . Hence DNS has been confined for now to the calculation of relatively low Reynolds number flows.

To circumvent these problems introduced by the wide range of temporal and spatial scales of turbulent flow many people resorted to a key characteristic in order to model it cost effectively; the fact it reaches a statistical steady state when averaged over time. This led to a method involving the application of Reynolds averaging on the NSE producing the well-known RANS. Considering an arbitrary quantity ψ , its average in time can be defined as

$$\frac{1}{T} \int_1^T \psi(\tau) d\tau$$

where the duration of time interval T must be much longer than that of the largest time scale in the flow. The RANS equations obtained describe the evolution of the mean quantities of the flow, thus generally regarded as a statistical approach, whereas the effect of the turbulent fluctuations appear in a Reynolds stress term (convection term in the momentum equation) which needs to be modeled in order to close the system. The turbulent models used here usually represent an approximate effect of turbulence on the mean flow quantities. NSE its low computational requirements and the fact that most engineering applications require knowledge only in the time average sense, RANS has been the most popular method used in CFD to date. It has found wide spread use in industry cause of its numerical simplicity and the small computational time required to achieve convergence when compared to the other two methods. But calculation of a turbulent (unsteady) flow using RANS definitely sounds contradictory to begin with. Explaining further, the RANS

approach assumes that the flow is statistically steady or at least the time scale of the unsteady motion is substantially larger than that of the turbulent motion [8, 9]. For the later condition, turbulent flows that meet such a requirement are indeed rare. The technique used in this case for closure is inevitably the same as the one used in the steady-state case since the origin of the problem remains similar.

Turbulence modelling in RANS tries to provide closure relations for the Reynolds stresses by relating them to known or determinable quantities such as strains, geometric parameters and flow scales in an approximate manner. This is achieved by using results obtained from experiment or DNS calculations for the stress-strain relationship and therefore, in effect, causes RANS turbulent modelling to be "dependent" on these results for the calculation of its unknown quantities. For this reason, RANS is regarded as a less universal approach compare to DNS and LES. The use of a single turbulence model to describe a wide range of turbulent scales is subject to scrutiny. Whereas small scales tend to depend entirely on viscosity, and could be located throughout the flow, the large ones are strongly affected by the boundary conditions and depend mostly on inertia. Thus it does not seem possible to model the effect of the large scales of turbulence in the same way in flows that are different. Also it is worth mentioning that RANS eddy-viscosity turbulent models are purely dissipative, do not predict backscatter and it's solution at any one instance is not time-accurate but time-average. There have been numerous reviews fairly recently, [10, 11] for example, that investigated the performance of a number of turbulence models employed in RANS, ranging from simple one or two equation linear eddy-viscosity models to nonlinear eddy-viscosity and Reynolds-stress models. It has been recognised that complex flows such as flows with separation and strong vortical features present, cannot be resolved. Thus one can say that the accuracy of the results obtained for such flows using RANS cannot be regarded as reliable. To extend the argument against the accuracy of RANS, there has been further research [12] into the negative effect the discretisation of the advective terms causes onto the numerical accuracy of RANS.

LES can be considered as a mid-point between DNS and RANS. In traditional LES, the variables of the NSE go through a predefined 'filtering' process which separates the turbulence into two distinct areas: that constituting of large scale components and that of smaller. Filtering is used to ensure that the velocity fields contain only the largest eddies from the turbulent field. This results in a system of equations referred to as the LES equations for the large scales. Large scale turbulence is computed directly without the need of any turbulence models since it is resolved by the modified (filtered) set of the

NSE. On the other hand a turbulence model is required for the smaller scale flow and, in the case of LES, this is achieved by using a Sub-Grid-Scale (SGS) model. So the LES approach deals with the complexity of resolving the large energy-carrying structures to momentum and energy transfer exactly just as in DNS, whereas similarly to RANS the effect of the smallest scales of turbulence is modeled. Moreover, LES must at the same time deal with the interactions between the two scales, that is making sure the energy cascade from the captured large scales to the small modelled scales is smooth.

In order to derive the LES equations, it is assumed that filtering and differentiation commute [13, 14], that is $\widehat{\partial f / \partial x} = \partial \widehat{f} / \partial x$, where the 'widehat' denotes the filtering process. But this relationship stands true only if the filter length is constant [15]. Additionally, due to the nonlinear system of equations, decomposition unavoidably leads to the appearance of additional terms during the filtering process since the components of the relevant equations cannot be written as exact and hence subgrid Reynolds stresses have to be included. As a result the closure problem appears again and the use of a SGS model is dictated.

Errors in LES arise due to the discrete representation of the NSE variables, numerical discretisation, aliasing and SGS modelling. The errors from the numerical discretisation are generated once the partial differential operators are replaced by numerical approximations. Truncation error analysis has shown that numerical discretisation leads to dispersive and dissipative terms. The dispersive terms are responsible for the oscillations noticed near a flow discontinuity, such as a shock, and the dissipative terms are responsible for the numerical dissipation. Also, SGS modelling is another source of error and difficulties. It is highly possible that the truncation error originating from the numerical discretisation could mask the SGS model [16] and hence the effects the truncation error has on the computed flow require prior knowledge.

The difference between DNS and RANS in modelling the turbulent scales can easily be given by a simple photography 'trick'. When taking a picture of a turbulent motion such as that in a river Figure 1.3(a), one can change the camera's shutter speed (measured in seconds of exposure, thus the faster the shutter speed the smaller the timeframe Δt). If the shutter speed is sufficiently small so that the quickest eddy motion has barely moved within that time frame, a *time accurate* visualisation of the flow is obtained, Figure 1.3(a). On the other hand, if the shutter speed is sufficiently large so that the slowest eddy can complete a number of rotations, a *time average* visualisation of the flow is obtained such as in Figure 1.3(b). The principle is similar to the difference of DNS and RANS turbulent

modelling. The first solves all scales in a time accurate fashion, whereas the latter solves the turbulent scales of the NSE in a time average sense, that is the contribution of the dissipation introduced by the turbulent scales is a time average value.



(a) Small shutter speed

(b) Large shutter speed

FIGURE 1.3: Unsteady river flow at different camera shutter speeds [3]

In LES, one can imagine the smaller scales of turbulence being modelled in a similar manner as to RANS (Figure 1.3(b)) whereas the larger scales are captured in the time accurate manner as in DNS (Figure 1.3(a)). Thus LES is a turbulence modelling method that employs the time accurate advantage of DNS while not being as computationally costly by employing a turbulence model for the SGS similar to RANS. However the way the SGS should be modelled for LES is not clear since the schemes used to solve the NSE may introduce errors due to approximations, discretisation e.t.c. that effect the numerical solution to a greater degree and thus need to be investigated first. Such a method that has been given a lot of interest over the past decade in the CFD community are high-resolution numerical methods for turbulent flows which have been speculated to have an embedded turbulence model capable of replacing the need for a SGS model as found by [17, 18], [19, 20, 21], [22, 23], [24, 25], and various others [26, 27, 28]. To extend the argument, it is believed that high resolution methods can accurately reproduce the effects of viscosity as well as a lot of the SGS-model properties. Hence a new kind of turbulence modelling within the LES context appeared, that of **Implicit-LES (ILES)**. The first to imply that there exists a coupling between the numerical properties of a high-resolution method and an intrinsic turbulence model was [29] and [30]. In ILES the SGS model is implicitly introduced by carefully designing the truncation error to look similar to that of an SGS

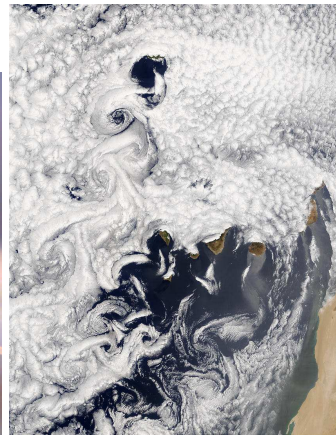
model by using high-resolution monotone algorithms for the convection discretisation of the unfiltered NSE. Since no additional equations for an SGS model are required, the numerical method is computationally less demanding.

Although development of new and more accurate models for the unresolved scales has allowed the simulation of flows in more complex configurations than previously possible, the application of LES to actual configurations of engineering interest hinges on the development of more efficient methodologies to represent the region near solid boundaries.

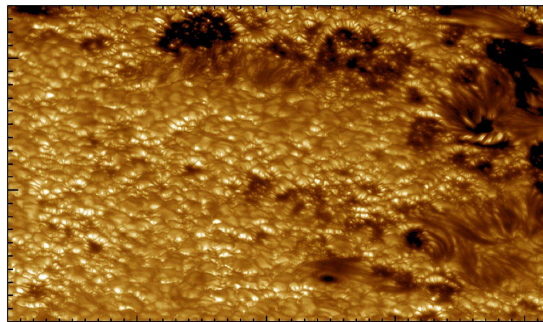
The appearance of turbulence spans across a wide range of scientific importance, from engineering Figure 1.4(a) to weather forecasting Figure 1.4(b) and even cosmic scales such as astrophysics Figure 1.4(c).



(a) Wing tip vortices of plane takeoff [31])



(b) Vortex sheet cloud formation over the Canary Islands [32]



(c) Turbulent flow on Sun's surface [33]

FIGURE 1.4: Turbulence in different scientific areas

Thus it's correct modelling is of great importance. However, more simple geometries have to be investigated initially before applying it to any more complex simulation scenarios. A channel flow is an excellent problem to use to investigate the properties of a SGS model near a wall. The presence of a solid boundary tends to alter the behaviour of the turbulent flow in a number of ways that need to be modeled by the SGS model in order to correctly represent the flow near the wall and most importantly capture the boundary layer. It also inhibits the growth of the small scales, alters the exchange mechanisms between the resolved and unresolved scales and finally gives rise in the SGS near wall region to important Reynolds-stress producing events. The accuracy of the SGS model in modelling correctly the under-resolved turbulent flow near the wall is important for various of today's engineering design procedures as for example in lifting bodies and wings where important properties such as the coefficient of friction and lift depend primarily on the correct resolution of the boundary layer.

Plane channel flow has been used as a test case throughout the literature cause it allows clear interpretation of the turbulent modelling ability of a numerical scheme. It's simple domain, without any geometrical gradients, means that the creation and sustainability of turbulence at a certain Reynolds number will clearly depend on the numerical scheme's turbulent modelling ability. As discussed in [34] channel flow is one of the three major 'canonical' flows being used by researchers to perform stringent tests and detailed validation of LES methods. Incompressible DNS results are widely available with [35] being the most widely used as reference data for comparing obtained LES results. LES investigations of channel flow can be primarily distinguished depending on the modelling approach of the near wall region that they employ.

In [36, 37] DES is used. The approach used RANS turbulence modelling in the near wall region and ILES in the remaining domain giving a good law of the wall. In [38] explicit LES filtering with SGS models is used alongside wall-functions in the near wall region. The results obtained were good in terms of the resolution of the velocity and turbulence intensities away from the wall for over 80% of the channel width. Literature on traditional LES using filtering and investigating various SGS models is numerous, [39, 40, 41] to name a few, with most reporting positive results in the resolution of mean velocity and velocity fluctuation profiles. Incompressible ILES investigations have also been recently conducted in [20, 21, 42] in which it was demonstrated that ILES managed to reproduce first and second order statistical moments of the velocity field better than filtered LES using isotropic eddy-viscosity SGS models.

Experimental results are also scarce due to the difficulties in measuring quantities in turbulent flows with only a few conducted [43, 44, 45], all at low Reynolds numbers using either water or oil as a medium thus incompressible. In [44], a DNS and experiment were conducted at the same Reynolds number and compared. It was observed that good agreement was obtained between LDV measurements of velocity RMS and Reynolds shear stress. This provides assurance about the accuracy of the measurements and the reliability of the DNS in whole when being used to validate against. The agreement between calculations and measured values of the flatness and skewness agree within the ability to correct for noise that is generated during the experiment's data acquisition process. In [43], measurements were obtained of the mean velocity, the Reynolds stress, the mean-square of the streamwise and normal velocity components, and the skewness and flatness of the fluctuating velocity components. The comparison with DNS showed a very close agreement between the measurements of the mean-square of the normal velocity fluctuations, removing problems that existed in a previous comparison ([46]) with hot-wire or hot-film measurements. The small, but significant, differences noted with the streamwise velocity fluctuations suggest that more nodes or a larger computational domain in the flow direction would slightly improve the computation.

Compressible channel flow literature is much less extensive and in fact rare in spite of its engineering importance. DNS results are restricted only to a few cases, most noticeable being [47, 48, 49]. This is primarily due to the higher computational costs required to solve the nonlinear terms, more than 50% and 85% as reported in [50, 51] respectively, rising from the use of more complex numerical schemes employed due to boundary condition modelling issues [49]. LES investigations of compressible channel flow are also just a few. In [52] a multilevel algorithm is used to speed computations and help compute SGS terms for coarser grids on which the solution is obtained and results give good agreement with the sub-grid terms extracted from filtered DNS. Other LES investigations of compressible turbulent boundary layer include [53, 54, 55] from which the latter interestingly includes shock-boundary layer interactions. One of the few compressible ILES investigations conducted was [56] carried out in a configuration corresponding to a bluff body flow in a rectilinear duct. Various models were analysed including eddy viscosity, scale similarity, mixed and dynamic models and finally the concept of monotone integrated large eddy simulation MILES. Note that MILES is now considered part of a greater range of methods called ILES. It was found that the results from the numerical simulations were fairly resilient to the SGS models selected when the computational grid was fine enough.

This investigation concerns with looking into the ability of ILES in simulating flow behaviour in under-resolved, compressible, turbulent flows with emphasis to the near-wall region. Initially a comparison will be made between results obtained using various high-resolution methods and those obtained from DNS. This will be achieved by using a fully developed turbulent channel flow as a test case. The relationship between individual terms as appear in the design of high resolution schemes and the numerical dissipation and dispersion will be examined for both compressible and incompressible regimes. Further on, different variants of flux limiters and high-resolution/higher-order schemes will be implemented, their properties assessed and those performing best utilised in simulating supersonic flows.

The aerospace industry is one of the most predominant areas that deal with supersonic flows. Usually the formation of a shock wave over an aerodynamic section leads to a number of other complex fluid phenomena such as a detached boundary layer and shock-boundary layer interaction. This can result to unusual wave patterns such as λ shockwaves as seen in Figure 1.5. Such phenomena require the use of shock-capturing schemes while at the same time being able to model turbulence adequately. Fortunately, high resolution methods are regarded as shock-capturing methods and within the ILES framework, their ability to capture turbulence correctly is also investigated.

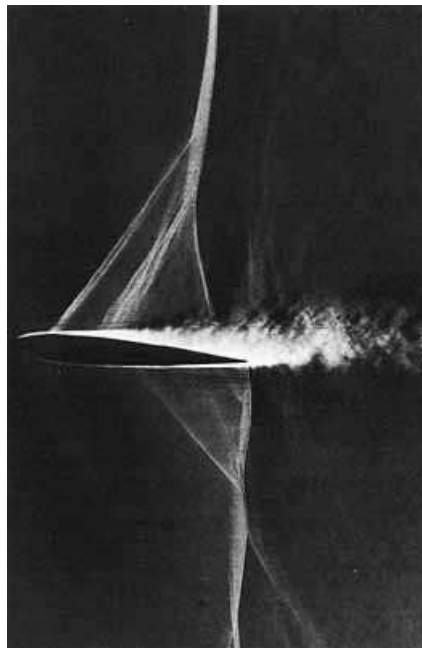


FIGURE 1.5: λ shocks and boundary layer-shock wave interaction on airfoil profile NACA 0012, Schlieren visualisation. [4]

Most practical applications of numerical modelling encountered in aerodynamics and generally in a lot of engineering applications, require a compressible flow description. For this reason a test case is also selected to examine this flow regime too. At mentioned earlier, high Mach number flows often exhibit strong unsteady flow phenomena which cannot be properly predicted by RANS solutions.

In [57] and [58] the status of RANS simulations was summarised for compression corner flows. It was observed that no RANS model was capable of accurate prediction of all aspects of the flowfield. Specifically, the RANS solutions did not display the unsteadiness of the separation shock, which was regarded as a major flaw and the source of the disagreement with the experimental mean surface pressure. On the other hand, the use of DNS in high Mach number flows at the current point in time is in practise to industry infeasible, firstly due to the high Reynolds numbers one may come across and/or secondly due to the more relatively prohibiting complex geometries. On the other hand it is possible to apply LES on much coarser meshes than DNS while at the same time being time accurate unlike RANS. The advantage of LES over RANS in this case is the fact that strong unsteady flow phenomena experienced in high Mach number compressible flows require a time accurate solution. However, most effort put into developing SGS models for LES has been conducted for incompressible solvers and has resulted in just a few designed for compressible SGS models. Thus the applicability of ILES for turbulence modelling in this turbulent supersonic compressible flow regime will be examined.

In [59] ILES was also employed to compressible isotropic turbulence and it was concluded that the influence of the numerical dissipation is considerable and most shock-capturing schemes examined were unable to mimic the SGS dissipation correctly. However, it was also recommended to avoid using any SGS turbulence model on the grounds that the numerical dissipation of the schemes is larger than the dissipation added by a SGS and is therefore 'masked' in any case. The investigation in [59] did not cover viscous fluxes or inhomogeneous turbulence and made no attempts to improve on the results by introducing any numerical treatment. A wide list of cases for simulating such compressible flows can be found in [60] where the literature survey conducted was exhaustive resulting with a plethora of cases and configurations.

From the available options, a compression ramp is proposed as an investigative case which can be thought of as a deflected flap. This is a standard CFD validation case for shock wave turbulent boundary layer interaction. The flow consists of an equilibrium

supersonic turbulent boundary layer of thickness δ approaching a compression corner defined by an angle α_{cc} . The deflection of the flow by the corner generates a shock system which for a sufficiently large pressure rise, the boundary layer separates and a λ -shock forms. This is in direct relationship to the shock pattern featured over the aerofoil in Figure 1.5 and constitutes the compression ramp as a valid case to investigate the numerical abilities of a method in modelling such phenomena before being applied to more complex geometries.

In [61] distinction is made between various types of pressure rise associated with separated flow, and an opinion is given as to their significance for design purposes. Only turbulent separations are considered and further, only three types of pressure rise are distinguished. These are

1. The pressure rise to the separation point of a flow already separated,
2. the first peak pressure rise in a flow already separated,
3. the over-all pressure rise for incipient separation for a flow for-which the boundary layer is just on the verge of separation

The pressure rise to separation likely would not be of interest to a designer, but would be to a research worker concerned with the mechanism of turbulent separation. The first peak pressure rise, on the other hand, would be of interest to a designer concerned with loads, hinge moments, or flap effectiveness. The over-all pressure rise for incipient separation would be of interest to a designer who does not want a flow to separate, yet wants to achieve the maximum pressure rise possible, such as is the case for inlet design. One pressure distribution, corresponds to a flap deflection which produces a separated flow. The other flow condition, corresponds to a somewhat smaller flap deflection for which there is no appreciable separated region, but for which the flow is just on the verge of separating.

In [62] the longitudinal pressure distribution for compression corners has been studied over a range of Mach and Reynolds numbers to determine the test conditions for the initial appearance of the pressure-distribution curve with three inflection points. In the ensuing discussion, example pressure distributions will be shown for the three model types investigated and the resulting points of incipient separation will be discussed as a function of Mach number, Reynolds number and model shape. From the results it can be determined whether a compression corner under selected conditions will develop incipient separation or not.

In [63] the relationship between incoming boundary-layer properties and the unsteadiness of a shock-induced separated flow was examined. A large quantity of Particle Image Velocimetry (PIV) data was obtained in the boundary layer just upstream of the interaction simultaneous with fluctuating wall pressure measurements beneath the unsteady separation shock foot. Ensemble average velocity profiles derived from the PIV data were computed, conditioned on the instantaneous location of the separation shock foot within the intermittent region, as derived from the wall pressure measurements. Mean velocity profiles for shock-upstream and shock-downstream positions found no difference in the boundary-layer thickness with shock position, in agreement with previous planar laser imaging experiments. This suggested that the thickening/thinning of a boundary layer is probably not the cause of shock unsteadiness. Ensemble average velocity fluctuations conditioned on different types of separation shock foot motion showed that although no significant distinction was apparent in the outer region of the boundary layer, nearer to the wall, positive velocity fluctuations correlated with downstream shock motions and vice versa. Furthermore, larger fluctuations corresponded to longer shock excursions. These observations are consistent with the physical principle wherein a momentarily fuller velocity profile imparts greater resistance to separation to the boundary layer and, hence, induces a downstream shock motion and vice versa. These results are the first to offer direct experimental evidence of a relationship between the velocity fluctuations in the upstream boundary layer and the motion of the separation shock foot.

In [64] high-speed PIV measurements were performed in streamwise-spanwise planes of a shock-wave turbulent boundary layer interaction generated by a 20° ramp in a Mach 2 flow. Velocity fields of the upstream boundary layer in the log region ($y/\delta = 0.2$) reveal elongated regions of low- and high-speed fluid that extend to streamwise lengths greater than 30δ (length computed based on Taylor's hypothesis). The velocity signature is remarkably similar to the signature observed in incompressible boundary layers. The presence of elongated regions of uniform momentum in the velocity fields also validates the use of planar laser scattering data as a qualitative marker for velocity. High-speed PIV measurements of the interaction capture a considerable part of the upstream boundary layer and the separation region upstream of the compression ramp. Time sequences of instantaneous velocity fields show the presence of long regions of uniform momentum (both high- and low-momentum) in the upstream boundary layer and the instantaneous spanwise separation line of the shock induced separation region is seen to be undulated, conforming to the presence of high- and low-speed regions in the upstream boundary

layer. Statistical analysis (i.e. correlations) and observations of various instantaneous velocity fields indicate that the location of separation is pushed downstream if the upstream boundary layer is faster. Conversely, the separation region is far upstream if the boundary layer is slower. Locally averaged sequences of the velocity fields (i.e. low-pass filtered) reveal a stronger correlation between the upstream boundary layer and the location of separation. This indicates that the small-scale velocity fluctuations in the boundary layer reduces the correlation between the large scale velocity fluctuations and the separation location. This lends further support to previous observations [65, 66], that elongated low- and high-speed regions in the boundary layer is a turbulent mechanism that can account for the low frequency unsteadiness of the shock induced separation region found in various shock-boundary layer interactions.

In this case, a number of other DNS and LES investigations are used to compare against and observations will be deducted from the results obtained. Further, Physical phenomena noticed in the literature will be attempted to be observed, however a quantitative comparison will not be possible due to the difference in Reynolds number, Mach number and/or ramp deflection angle used.

Aims and Objectives

The main aim of this thesis is to investigate the ability of different solution strategies for the governing equations based on high-resolution methods in modelling turbulence near the wall in both subsonic and supersonic flow regimes using a compressible solver. One of the most important criteria that quantify such an ability are turbulent velocity profiles along with other near wall parameters such as coefficient of friction and wall shear stress. Further, good estimates in the near wall region of the flow could be used as a sign that the energy cascade is modelled correctly or efficiently enough since this is where the smallest scales are usually present and which in effect require to be modelled by LES. No turbulence models are used since this class of numerical schemes provide a built-in SGS model that may offer a better approach than explicit treatments. Otherwise, as mentioned earlier, one can negate the reason of using an explicit turbulence model altogether due to the much larger dissipation introduced by the numerical methods themselves. This implicit ability of high-resolution methods to model turbulent flows arises from the truncation error of the wave-speed dependent terms (which are responsible for generating numerical dissipation), when applying Godunov-type discretisation methods. It is essential to improve

the current understanding of the mechanisms that add dissipation to the flow through the truncation error and avoid over-dissipative numerical solutions by triggering entropy production where and when required.

The objectives can be summarised as follows:

- To assess the accuracy of different high resolution methods against detailed DNS and experimental data for basic near wall turbulent flows;
- To assess different variants of slope limiters and high resolution / higher order schemes;
- Examine new numerical methods to improve compressible turbulence modelling in low Mach number flows;
- Investigate the applicability and turbulence modelling capability of the limiters that prove the best in subsonic flows to those of supersonic.

Thesis Structure

The thesis is organised in three parts, each containing a number of chapters. The first part includes an introduction to the Ph.D. along with the necessary literature survey. In the second part, an overview of the theoretical and numerical framework employed is given. This is then finally followed by the third part which includes all the simulations conducted along with the discussion and any observations made of the results. The body of the thesis is thus structured as follows:

1. Part 1. Introduction - Here an introduction to the Ph.D. is made with the literature survey as part of the general description of the investigations conducted. To clarify, the underlining reasons and relevance to real flow scenarios are also mentioned.
2. Part 2. Theory - In this part all the necessary theoretical background, which includes the three-dimensional Navier-Stokes equations, and numerical methods are presented.
 - (a) Section 2.1 Theoretical Background - In this section all the physical equations used to describe the motion of fluids are presented;

- (b) Section 2.2 Numerical Background - A numerical version of the equations shown in the previous section are formulated and kept in a general finite volume form before applying any numerical methods;
 - (c) Section 2.3 Numerical Methods - Here the numerical methods used to obtain the results in the present thesis are applied to the general numerical form of the governing equations as shown in the previous section;
3. Part 3. Simulations and Results - Here the derived numerical methods are applied to a number of cases for analysis.
- (a) Section 3.1 Channel Flow - The ability of high resolution methods to model inhomogeneous turbulence is analysed in this section for relatively low Mach number flows;
 - (b) Section 3.2 Compression Ramp - In contrast to the low Mach number in the previous section, in this case the flow is turbulent, inhomogeneous and supersonic, thus expanding the range of the investigation of the turbulence capability of ILES even further;
 - (c) Section 3.3 Conclusions - Finally, the analysis of the results is summarised here, drawing out the main observations and based on those a few recommendations and guidelines are made for future work.

In addition, details related to the numerical scheme and any complementary material to the results presented are included in the appendices.

Theory

2

Theoretical Background

The Navier-Stokes equations may be obtained by using infinitesimal or finite control volume approaches, and the governing equations can be expressed in differential or integral forms. In Appendix B these equations are presented in differential form, and in Section 2.1 in integral form. For a detailed discussion of the derivation of these equations in either form, the reader is referred to [67] and for some core mathematical relationships used throughout the thesis to Appendix A.

2.1 Integral Form of Conservation Equations

The **Finite Volume Method (FVM)** is one of the most versatile discretisation techniques used in CFD. Based on the control volume formulation of analytical fluid dynamics, the first step in the FVM is to divide the domain into a number of control volumes (aka cells, elements) where the variable of interest is located at the centroid of the control volume. The next step is to integrate the differential form of the governing equations (very similar to the control volume approach) over each **control volume (CV)**. The conservation laws

presented above are integrated across a control volume as such shown in Figure 2.1. Interpolation profiles are then assumed in order to describe the variation of the concerned variable between cell centroids. The resulting equation is called the discretised or discretisation equation. In this manner, the discretisation equation expresses the conservation principle for the variable inside the control volume. The most compelling feature of the FVM is that the resulting solution satisfies the conservation of quantities such as mass, momentum, energy, and species. This is exactly satisfied for any control volume as well as for the whole computational domain and for any number of control volumes. Even a coarse grid solution exhibits exact integral balances. FVM is the ideal method for computing discontinuous solutions arising in compressible flows. Any discontinuity must satisfy the Rankine-Hugoniot jump condition which is a consequence of conservation. Since finite volume methods are conservative they automatically satisfy the jump conditions and hence give physically correct weak solutions. FVM is also preferred while solving partial differential equations containing discontinuous coefficients.

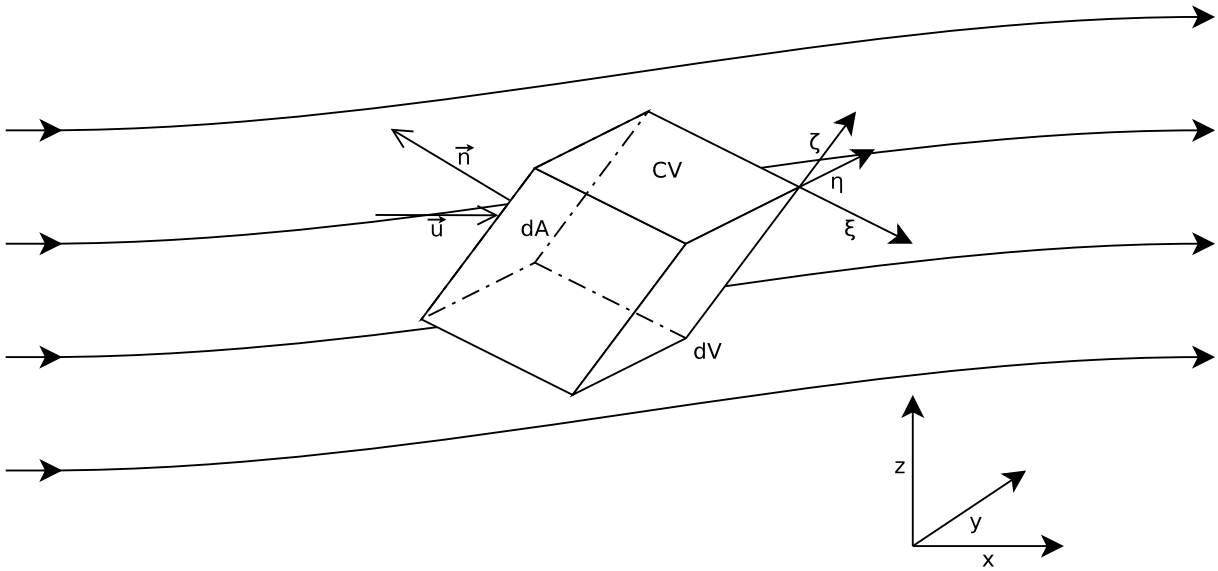


FIGURE 2.1: CV illustrated

Continuity

The continuity equation is based on the principle that

“Mass can be neither created nor destroyed”

Consider the finite control volume CV fixed in space, the flow velocity $\vec{u}$ and it's unit normal vector $\vec{n}$ corresponding to an elemental surface area dA of the CV. The time rate of the total mass inside the finite volume CV can be expressed mathematically as

$$\frac{\partial}{\partial t} \iiint_V \rho dV$$

The mass flow through a fixed surface dA is the product of density, surface area and it's perpendicular velocity component and is written as

$$\dot{m} = \rho \vee dA$$

Hence the contribution of the convective flux across each surface element can be expressed as

$$\rho \vec{u} \cdot \vec{n} dA = \rho \vec{u} \cdot d\mathbf{A}$$

The net mass flow out of the entire surface area is the summation over A of the elemental mass flow through dA . In the limit this becomes a surface integral

$$\oiint_A \rho \vec{u} \cdot d\mathbf{A}$$

Further considering that there are no volume or surface sources, Equation (B.1) can therefore be written in integral form as

$$\frac{\partial}{\partial t} \iiint_V \rho dV + \oiint_A \rho \vec{u} \cdot d\mathbf{A} = 0 \quad (2.1)$$

Momentum

The momentum equation is derived based on the principle that

“The force exerted on a body is equal to the time rate of change of momentum”

This is derived from Newton's second law that states that the force exerted on a body is equal to the body's mass times the acceleration due to the force. The time rate of change of momentum of the fluid as it sweeps through the fixed CV is the sum of two terms:

- Time rate of change of momentum due to unsteady fluctuations of flow properties inside V ;
- Net flow of momentum through the CV across surfaces of area A .

The momentum of an infinitesimally small portion (dV of the CV of volume V is simply given by

$$\rho \vec{u} dV$$

Thus the variation in time within the CV equals

$$\frac{\partial}{\partial t} \iiint_V \rho \vec{u} dV$$

The net flow of momentum through a volume element is equal to the accumulation of the momentum flow through all the volume's surfaces. The momentum flow crossing an elemental surface of area dA is given by

$$(\rho \vec{u} \cdot d\vec{A}) = \rho \vec{u} (\vec{u} \cdot \vec{n} dA)$$

Thus the net flow of momentum across the CV is the summation of all the above elemental surface areas

$$\oiint_A \rho \vec{u} (\vec{u} \cdot d\vec{A})$$

In the case of the CV as depicted in Figure 2.1 the possible forces acting on the surfaces as fluid flows through it are of two natures:

- *Body Forces*: such as gravity, electromagnetic forces or any other forces which “act at a distance” on the fluid inside the CV;
- *Surface Forces*: pressure and shear stress acting in the control surface A .

The body forces, $\vec{B}$, represent the net body force per unit mass exerted on the fluid inside V . The body force on the elemental volume dV is given by

$$\rho \vec{B} dV$$

and thus the total body force acting on the CV is given by the summation of the body forces acting on the elemental volumes across the CV of volume V

$$\iiint_V \rho \vec{B} dV$$

The elemental surface force due to isotropic pressure acting on the elemental area dA is

$$-pdA$$

where the negative sign is to indicate that the direction of the pressure force is opposite to that of $d\vec{A}$ or therefore of $\vec{n}$. So as similar to the body force above, the complete pressure force over the CV is given by

$$-\iint_A pdA$$

When viscous flow is considered, the shear and normal viscous stresses also exert a surface force. Their effect on the unit normal surface is given by

$$\bar{\bar{\tau}} \cdot \vec{n} dA$$

and, as done for the pressure, the complete force acting over the CV is given by

$$\iint_A \bar{\bar{\tau}} \cdot d\vec{A}$$

The form of the shear stress tensor, $\bar{\bar{\tau}}$, is elaborated in detail further in Section 2.3 where it is shown how the normal and shear stresses are connected to the velocity field. By using Newton's second law it is derived that the momentum of an infinitesimally small portion of the CV as shown in Figure 2.1 is given by

$$\rho \vec{u} dV$$

Thus the variation in time of momentum within the CV is expressed as

$$\frac{\partial}{\partial t} \iiint_V \rho \vec{u} dV$$

The contribution of the convective flux, which describes the transfer of momentum across the boundary of the control volume, to the conservation of momentum is then given by

$$-\oint\oint\oint_V \rho \vec{u} \cdot d\vec{A}$$

Applying all the above gives the momentum equation in integral form

$$\frac{\partial}{\partial t} \oint\oint\oint_V \rho \vec{u} dV + \oint\oint_A \rho \vec{u} (\vec{u} \cdot d\vec{A}) = - \oint\oint_A p d\vec{A} + \oint\oint_A \vec{\tau} \cdot d\vec{A} + \oint\oint\oint_V \rho \vec{B} dV \quad (2.2)$$

Energy

The energy equation is required with the implication though that it further introduces additional flow-field variables, the internal energy and temperature, which are discussed in Section 2.2. The energy equation is embodied in the first law of thermodynamics and thus the following principle holds true

"Energy can neither be created nor destroyed, it can only change in form"

When applied to the CV as displayed in Figure 2.1, it states that any change in time of the total energy inside the volume is caused by the rate of work of forces acting inside the volume and by the net heat flux through it. In turn, the total energy E per unit mass of a fluid is obtained by adding its internal energy e per unit mass, to its kinetic energy KE per unit mass

$$E = e + KE = e + \frac{\vec{u}^2}{2} = e + \frac{u^2 + v^2 + w^2}{2} \quad (2.3)$$

In this case the conserved quantity is the total energy-density or total energy per unit volume ρE . Its variation in time within the CV can be expressed as

$$\frac{\partial}{\partial t} \oint\oint\oint_V \rho E dV$$

The flux of the conserved quantity through the CV's surfaces is written as

$$-\oint\oint_A \rho E \vec{u} \cdot \vec{n} dA$$

The net heat flux comprises of two parts. The first is the heat flux due to volumetric rate of heat addition per unit mass due to absorption of radiation or emission of radiation, or due to chemical reactions and is denoted by $\dot{q}$. This term can also be seen as a heat transfer component due to mass diffusion. The mass contained within an elemental volume is ρdV and thus the rate of heat addition to this mass is $\dot{q}\rho dV$. The sum over the complete CV is thus

$$\iiint_V \dot{q}\rho dV$$

Heat can also be transferred into the CV by means of thermal conduction across the control surfaces due to temperature gradients. This is the second part of the net heat flux and in general is written in the form of Fourier's law of heat conduction

$$k\nabla T$$

where k is the thermal conductivity coefficient and T is the absolute static temperature. Thus the total net heat flux through the CV is

$$\iiint_V \dot{q}\rho dV + \iint_A k\nabla T dA$$

The rate of work of forces acting inside the volume comprises of two forces similar to as described in the momentum equation, those being the body forces and surface forces. The body forces are represented by $\vec{B}$ and as previously denotes the net force per unit mass exerted on the CV. The rate of work of the body force on an elemental volume dV is given by $\rho\vec{B}dV \cdot \vec{u}$. The total over the complete CV is thus given by

$$\iiint_V \rho\vec{B} \cdot \vec{u} dV$$

First of the surface forces experienced by the CV is pressure. Considering the pressure p acting on an elemental surface dA gives the pressure force experienced in the elemental volume equal to $-pdA$. Thus the rate of work done due to pressure acting on the elemental surface with a flow of velocity $\vec{u}$ passing through it is equal to $-pdA \cdot \vec{u}$. Summing

over the entire surface of the CV gives

$$-\oint\oint_A p \vec{u} \cdot d\mathbf{A}$$

The forces created on an elemental surface dA due to the stresses arising from the viscous nature of the flow can be written in terms of the stress tensor $\bar{\bar{\tau}}$ as $\bar{\bar{\tau}} \cdot d\mathbf{A}$ and thus the rate of work done is $(\bar{\bar{\tau}} \cdot \vec{u}) \cdot d\mathbf{A}$. Over the entire surface of the CV the rate of work due to the viscous stresses can thus be found by

$$\oint\oint_A (\bar{\bar{\tau}} \cdot \vec{u}) \cdot d\mathbf{A}$$

Thus the total rate of work of forces experienced by the CV is given by

$$\oint\oint\oint_V \rho \vec{B} \cdot \vec{u} dV - \oint\oint_A p \vec{u} \cdot d\mathbf{A} + \oint\oint_A (\bar{\bar{\tau}} \cdot \vec{u}) \cdot d\mathbf{A}$$

Putting all the above parts together results in the total density-energy equation formulation

$$\begin{aligned} \frac{\partial}{\partial t} \oint\oint\oint_V \rho E dV + \oint\oint_A \rho E \vec{u} \cdot d\mathbf{A} &= \oint\oint\oint_V \dot{q} \rho dV + \oint\oint_A k \nabla T dA + \\ &\quad \oint\oint\oint_V \rho \vec{B} \cdot \vec{u} dV - \oint\oint_A p \vec{u} \cdot d\mathbf{A} + \oint\oint_A (\bar{\bar{\tau}} \cdot \vec{u}) \cdot d\mathbf{A} \end{aligned} \quad (2.4)$$

2.2 Perfect Gas Formulations

When studying the full compressible NSE which includes as presented above the continuity, momentum and total energy equation, it is made obvious that there is not a sufficient number of equations to the number of variables in order to 'close' the system of equations and thus additional fundamental equations are required. These are obtained by examining the thermodynamic properties of the considered flow's substance. The NSE describe the motion of fluids, that is a collection of particles which are in more or less a constant random motion. Due to the electrical charge of some of these particles, a force field pervades the space around them called *intermolecular force*. However if the particles of the gas are far enough from each other then the influence of the intermolecular force is small and can be neglected. A gas which the intermolecular forces are neglected is defined as a *perfect*

gas. For a perfect gas the following relations hold:

Equation of State

$$p = \rho RT \quad (2.5)$$

, where R is the specific gas constant. Unfortunately the Equation of State (EoS) introduces a seventh unknown that of temperature T . Thus a seventh equation is required in order to achieve closure of the set of equations. This is achieved by using a thermodynamic relation between state variables and in this case the Caloric Equation of State by assuming a calorically perfect gas, that is the temperatures are moderate and thus the specific heats remain constant.

Diffusive Coefficients

The diffusive coefficients are comprised of the thermal conductivity k , and the viscous coefficients λ and μ which are related to the thermodynamic variables by means of kinetic gas theory. Several of the assumptions on which their derivation is based are semi-empirical in nature. A detailed account of their derivation is given by Schliting [68]. It is possible to compute the Prandtl Number Pr , which is defined as

$$Pr = \frac{\mu c_p}{k} \quad (2.6)$$

where c_p is the specific heat at constant pressure. For more details see Appendix A.2.

Sutherland's Law

A conventional relation for the temperature variation of μ for air is given by Sutherland's law,

$$\frac{\mu}{\mu_0} = \left(\frac{T}{T_0} \right)^{3/2} \frac{T_0 + S_u}{T + S_u} \quad (2.7)$$

where T and S_u are in kelvin and μ_0 is a reference viscosity at a reference temperature T_0 . In most cases the reference values for viscosity and temperature are taken at standard atmospheric conditions at sea level then $\mu_0 = 1.7894 \times 10^{-5} \text{ kg/(m} \cdot \text{s)}$ and $T_0 = 288.16 \text{ K}$. Also the Sutherland temperature is taken as $S_u = 110.4 \text{ K}$.

Further Equations

For a specific gas, the specific heats at constant pressure c_p and constant volume c_v are related by

$$c_p - c_v = R$$

where R is the gas constant equal to $287.05 \text{ J/kg}\cdot\text{K}$ and

$$\gamma = \frac{c_p}{c_v}$$

where γ is the specific heat ratio and equals 1.4 under standard atmospheric conditions.

Also they are defined as

$$c_p = \frac{\gamma R}{\gamma - 1}$$

and

$$c_v = \frac{R}{\gamma - 1}$$

For air at standard conditions the following are implied:

$$\gamma = 1.4$$

and

$$R = 287 \text{ J/(kg} \cdot \text{K)}$$

The total density-energy is then given by

$$\rho E = \rho e + \frac{\rho}{2} (u^2 + v^2 + w^2) \quad (2.8)$$

where e stands for the internal energy. The caloric equation of state is used in order to calculate the internal energy

$$e = c_v T = \frac{RT}{\gamma - 1} = \frac{\rho RT}{\rho(\gamma - 1)} = \frac{p}{\rho(\gamma - 1)} \quad (2.9)$$

where c_v is the specific heat at constant volume, e is the internal energy and T is the absolute temperature.

2.3 Shear and Normal Stresses

The viscous stresses arise due to the friction between the fluid and the surface of an element and is described by the stress tensor $\bar{\bar{\tau}}$. In Cartesian coordinates the general form is given as

$$\bar{\bar{\tau}} = \begin{bmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{bmatrix} \quad (2.10)$$

where the first subscript character denotes the axis at which the plane is perpendicular to and the second the direction of the stress on that plane as shown below in Figure 2.2. Stresses with identical characters in their subscript denote normal stresses whereas otherwise denote shear stresses.

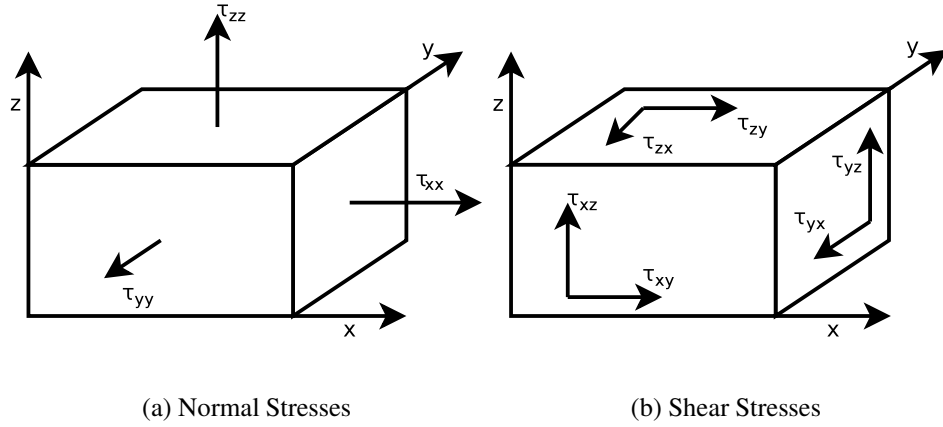


FIGURE 2.2: Stresses acting on CV

The computation of the shear stresses depends on the dynamical properties of the medium considered. Assuming air, Isaac Newton stated that the shear stress is proportional to the velocity gradient. Hence a fluid of such attribute is referred to as a *Newtonian Fluid*. For a Newtonian fluid such as air the components of the **viscous** stress tensor (as derived by George Stokes) are given by the following relations

$$\tau_{xx} = \lambda \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) + 2\mu \frac{\partial u}{\partial x}$$

$$\begin{aligned}
\tau_{yy} &= \lambda \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) + 2\mu \frac{\partial v}{\partial y} \\
\tau_{zz} &= \lambda \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) + 2\mu \frac{\partial w}{\partial z} \\
\tau_{xy} &= \tau_{yx} = \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \\
\tau_{xz} &= \tau_{zx} = \mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \\
\tau_{yz} &= \tau_{zy} = \mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)
\end{aligned}$$

where λ represents the second viscosity coefficient and μ denotes the dynamic viscosity coefficient. In order to close the expressions of normal stresses, Stokes introduced the hypothesis that the sum of the normal stresses is zero in order for the CV to be in equilibrium and therefore deduced

$$\lambda = -\frac{2}{3}\mu \quad (2.11)$$

Applying Equation (2.11) to the normal stresses gives

$$\begin{aligned}
\tau_{xx} &= 2\mu \left(\frac{\partial u}{\partial x} - \frac{1}{3} \nabla \cdot \vec{u} \right) \\
\tau_{yy} &= 2\mu \left(\frac{\partial v}{\partial y} - \frac{1}{3} \nabla \cdot \vec{u} \right) \\
\tau_{zz} &= 2\mu \left(\frac{\partial w}{\partial z} - \frac{1}{3} \nabla \cdot \vec{u} \right)
\end{aligned} \quad (2.12)$$

2.4 Complete System of the NSE

In the previous sections, we have separately derived the conservation laws of mass, momentum and energy. Now, we can collect them into one system of equations in order to obtain a better overview of the various terms involved. For reasons to be explained later, two flux vectors are introduced, namely $\vec{F}_c$ and $\vec{F}_v$. The first one, $\vec{F}_c$, is related to the convective transport of quantities in the fluid. It is usually termed vector of convective fluxes, although for the momentum and the energy equation it also includes the pressure terms $p\vec{n}$ (Equation (2.2)) and $p(\vec{u} \cdot \vec{n})$ (Equation (2.4)), respectively. The second flux

vector - vector of viscous fluxes $\vec{F}_v$, contains the viscous stresses as well as the heat diffusion. Additionally, a source term $\vec{Q}$ is defined, which comprises all volume sources due to body forces and volumetric heating. With all this in mind and conducting the scalar product with the unit normal vector $\vec{n}$, we can cast Equation (2.1), Equation (2.2) and Equation (2.4) into

$$\frac{\partial}{\partial t} \iiint_V \vec{W} dV + \iint_A (\vec{F}_c - \vec{F}_v) dA = \iiint_V \vec{Q} dV \quad (2.13)$$

The vector of the conservative variables $\vec{W}$ consists in three dimensions of the following five components

$$\vec{W} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix} \quad (2.14)$$

For the vector of convective fluxes

$$\vec{F}_c = \begin{bmatrix} \rho \vee \\ \rho u \vee + n_x p \\ \rho v \vee + n_y p \\ \rho w \vee + n_z p \\ \rho E \vee \end{bmatrix} \quad (2.15)$$

Where $\vee$ is the contravariant velocity, that is the velocity normal to the surface element dA defined as the scalar product of velocity vector and the unit normal vector

$$\vee = \vec{u} \cdot \vec{n} = n_x u + n_y v + n_z w$$

The total density-energy is given by Equation (2.8). The vector of viscous fluxes, $\vec{F}_v$ is

given by

$$\vec{F}_v = \begin{bmatrix} 0 \\ n_x \tau_{xx} + n_y \tau_{xy} + n_z \tau_{xz} \\ n_x \tau_{yx} + n_y \tau_{yy} + n_z \tau_{yz} \\ n_x \tau_{zx} + n_y \tau_{zy} + n_z \tau_{zz} \\ n_x \Theta_x + n_y \Theta_y + n_z \Theta_z \end{bmatrix} \quad (2.16)$$

where

$$\begin{aligned} \Theta_x &= u\tau_{xx} + v\tau_{xy} + w\tau_{xz} + k\frac{\partial T}{\partial x} \\ \Theta_y &= u\tau_{yx} + v\tau_{yy} + w\tau_{yz} + k\frac{\partial T}{\partial y} \\ \Theta_z &= u\tau_{zx} + v\tau_{zy} + w\tau_{zz} + k\frac{\partial T}{\partial z} \end{aligned} \quad (2.17)$$

are the terms describing the work of viscous stresses and the heat conduction in the fluid.

3

Numerical Background

In this chapter the numerical procedure's steps taken are shown and the relevant physical formulae are treated as such to make them possible to calculate numerically using various methods as detailed in Chapter 4.

3.1 Non-Dimensionalised Governing Equations

Before using any numerical methods it is best to non-dimensionalise the governing equations first. For this the vector variable form of the conservation equations is used, see Section 2.4. Consider non-dimensionalisation based on some characteristic values (subscript c). For consistency, in this section all variables without dimensions have * superscript and all values with dimensions have no superscript. Then dimensionless values are given by:

$$t^* = \frac{t}{\frac{l_c}{u_c}}, \quad (x^*, y^*, z^*) = \frac{(x, y, z)}{l_c} \quad (3.1)$$

$$\rho^* = \frac{\rho}{\rho_c}, \quad \mu^* = \frac{\mu}{\mu_c}, \quad (u^*, v^*, w^*) = \frac{(u, v, w)}{u_c} \quad (3.2)$$

$$\tau^* = \frac{\tau}{\frac{\mu_c u_c}{l_c}}, \quad p^* = \frac{p}{\rho_c u_c^2} \quad (3.3)$$

$$T^* = \frac{T}{T_c} \quad (3.4)$$

Substituting Equation (3.1) to Equation (3.4) in Equation (2.13) gives

$$\frac{\partial}{\partial t} \iiint_V \vec{W} dV + \iint_A \left(\vec{F}_c - \frac{1}{Re} \vec{F}_v \right) dA = \iiint_V \vec{Q} dV \quad (3.5)$$

where the Reynolds number Re is defined by

$$Re = \frac{\rho_c u_c l_c}{\mu_c}$$

For simplicity, the * superscript will be dropped in dimensionless quantities henceforth. Exact details of the non-dimensionalisation can be found in Appendix D.1.2.

3.2 Geometrical Quantities of a CV

Before continuing into the details of the numerical methods it is useful to first consider at this point the calculation of some geometrical quantities that arise in the NSE due to their discretisation onto the CV. Those are the CV's volume $V_{i,j,k}$, the unit normal vector $\vec{n}$ and the area ΔA of a face a . Further, the normal vector and face area are also known as the *metrics* of the CV. The calculation of face vectors and volumes hides some problems however in the case of a 3D (three-dimensional) cell. The origin of the problem comes from the fact that the four vertexes of a cell's face may not lie in the same plane, as represented in Figure 3.1. Then the normal vector is no longer a single constant property of the face.

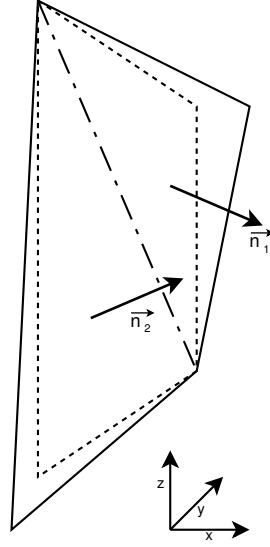


FIGURE 3.1: Two normal vectors for a face's surface

A way to treat this problem would be to decompose all six faces of the CV to two or more triangles each resulting in a volume made up of tetrahedra. Thus all the geometrical values could be calculated on the tetrahedra and then summed for the CV. However this would increase the computational load considerably since the fluxes would have to be calculated at the additional faces and integrated over each partial triangle separately resulting in the number of point operations to be double at the least. For smooth grids the CV's faces approach parallelograms and the decomposition into triangles does not noticeably increase the solution accuracy. Hence a simplified formulation for the computation of the quadrilaterals face areas is employed which is based on the averaged normal vector or otherwise the absolute value of the vector cross product. A face vector $\vec{A}$ based on a vector like that of $\vec{n}_1$ in Figure 3.3 can be computed using Gauss's formula. First we discretise the face vector $d\mathbf{A}$ as follows:

$$d\mathbf{A} = \vec{A} = \vec{n} dA = \vec{n} \Delta A$$

Note that ΔA is an area of a CV's face and is computed by the quadrilateral's diagonals cross product as shown in Figure 3.2 and formulated as:

$$\Delta A = \frac{1}{2} \left| \vec{f} \times \vec{g} \right| \quad (3.6)$$

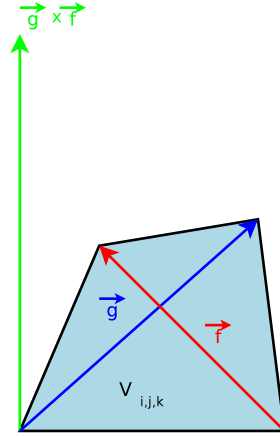


FIGURE 3.2: Quadrilateral's diagonal vectors cross product

In matrix form Equation (3.6) can be written as:

$$\Delta A = \frac{1}{2} \begin{vmatrix} i & j & k \\ \Delta x_{\vec{f}} & \Delta y_{\vec{f}} & \Delta z_{\vec{f}} \\ \Delta x_{\vec{g}} & \Delta y_{\vec{g}} & \Delta z_{\vec{g}} \end{vmatrix} \quad (3.7)$$

For face $m = 1$ in Figure 3.3, some differences are first defined:

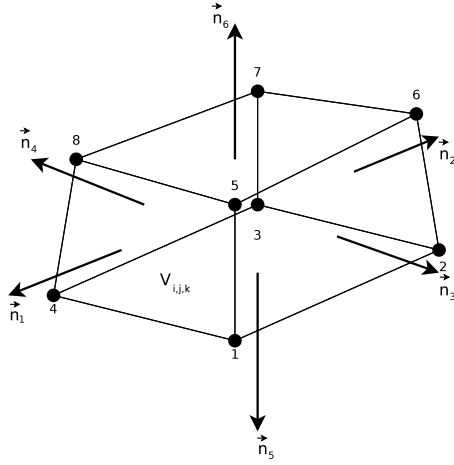
$$\Delta x_A = x_8 - x_1, \Delta x_B = x_5 - x_4$$

$$\Delta y_A = y_8 - y_1, \Delta y_B = y_5 - y_4$$

$$\Delta z_A = z_8 - z_1, \Delta z_B = z_5 - z_4$$

The face vector $\vec{A}_1 = \vec{n}_1 \Delta A_1$ results then from

$$\vec{A}_1 = \frac{1}{2} \begin{bmatrix} n_x & n_y & n_z \end{bmatrix} \begin{bmatrix} \Delta y_A \Delta z_B - \Delta z_A \Delta y_B \\ \Delta z_A \Delta x_B - \Delta x_A \Delta z_B \\ \Delta x_A \Delta y_B - \Delta y_A \Delta x_B \end{bmatrix} \quad (3.8)$$

FIGURE 3.3: CV and associated unit normal vectors (n_m) for a structured grid

Note that in Equation (3.8) there are three components. These stand for the area components normal to each axis as depicted below in Figure 3.4 in a 2D case for simplicity.

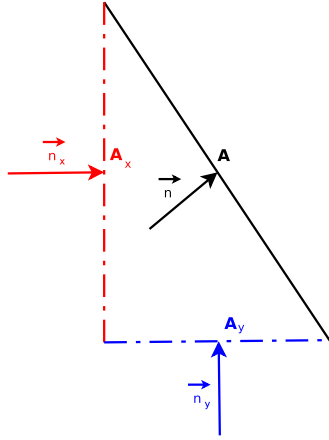


FIGURE 3.4: 2D surface normals

The remaining five surface vectors are calculated in a similar manner. However one may calculate three of the surfaces as long as they are perpendicular to each other and the remaining three surfaces equal to the appropriate neighboring CVs face's values but with reverse signs. The above expression in Equation (3.8) returns an approximate value for the face vector which becomes exact once the face approaches a parallelogram, that is when all the points lie in one plane. The unit normal vector is obtained from

$$\Delta A_m = \sqrt{A_{x,m}^2 + A_{y,m}^2 + A_{z,m}^2} \quad (3.9)$$

where

$$\vec{A}_m = \begin{Bmatrix} A_{x,m} & A_{y,m} & A_{z,m} \end{Bmatrix} = \vec{n}_m \Delta A_m$$

The last geometrical quantity to compute is the volume of each cell. The idea here is similar to that used to compute the area of the CV's surfaces, meaning that a vector cross product is used as shown in Figure 3.5. The formulation is usually referred to as a *scalar triple product*.

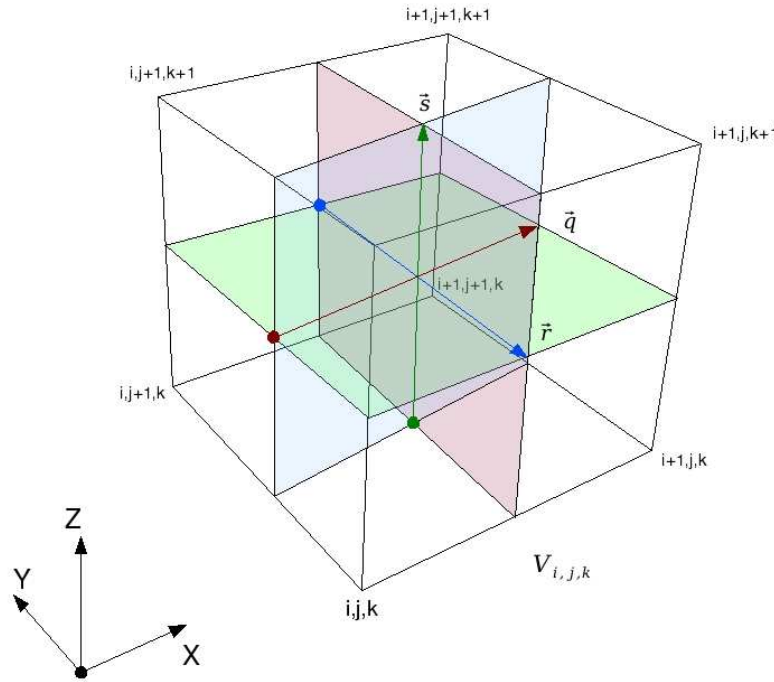


FIGURE 3.5: Cross vectors used to compute volume of CV

The formulation for the volume in vector notation is then given by:

$$\Delta V = \left| \vec{q} \cdot (\vec{r} \times \vec{s}) \right| \quad (3.10)$$

It is possible to write Equation (3.10) in matrix form as:

$$\Delta V = \begin{bmatrix} \Delta x_{\vec{q}} & \Delta y_{\vec{q}} & \Delta z_{\vec{q}} \\ \Delta x_{\vec{r}} & \Delta y_{\vec{r}} & \Delta z_{\vec{r}} \\ \Delta x_{\vec{s}} & \Delta y_{\vec{s}} & \Delta z_{\vec{s}} \end{bmatrix} \quad (3.11)$$

The componets of the matrix on the right hand side of Equation (3.11) are computed as:

$$\begin{aligned} \Delta X_{\vec{q}} &= \frac{X_{i+1,j,k} + X_{i+1,j+1,k} + X_{i+1,j+1,k+1} + X_{i+1,j,k+1}}{4} - \frac{X_{i,j,k} + X_{i,j+1,k} + X_{i,j+1,k+1} + X_{i,j,k+1}}{4} \\ \Delta X_{\vec{r}} &= \frac{X_{i,j+1,k} + X_{i+1,j+1,k} + X_{i+1,j+1,k+1} + X_{i,j+1,k+1}}{4} - \frac{X_{i,j,k} + X_{i+1,j,k} + X_{i+1,j,k+1} + X_{i,j,k+1}}{4} \\ \Delta X_{\vec{s}} &= \frac{X_{i,j,k+1} + X_{i+1,j,k+1} + X_{i+1,j+1,k+1} + X_{i,j+1,k+1}}{4} - \frac{X_{i,j,k} + X_{i+1,j,k} + X_{i+1,j+1,k} + X_{i,j+1,k}}{4} \end{aligned}$$

where $X = \{x, y, z\}$.

A detailed description which also includes mathematical derivations and/or proofs of the above methods in calculating the cell volume and surface areas can be found in [69].

3.3 Discretisation

The majority of numerical schemes for the solution of the Euler and NSE employ the method of lines, i.e., a separate discretisation in space and time. By consequence, it allows one to use numerical approximations of different accuracy for the spatial and temporal derivatives, as it may be required by the problem to be solved. Thus, a lot of flexibility is gained by this approach and is the very reason why the method of lines approach is implemented. A general, structured, finite volume scheme is naturally based on the conservation laws, which are expressed by the NSE Equation (3.5). In a pre-processing step, the physical space is subdivided into a number of grid cells - quadrilaterals in 2D, hexahedra in 3D. The resulting structured grid is uniquely described by the coordinates x, y, z of the grid points (corners of the grid cells) and indices (i, j, k) in the computational space (see Figure 3.6). Based on the grid, control volumes are defined in order to evaluate the integrals of the convective and viscous fluxes as well as of the source term.

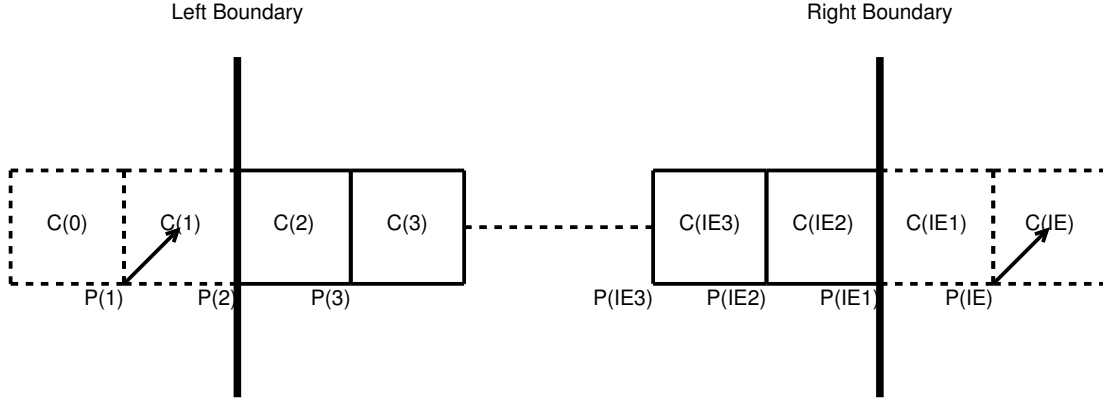


FIGURE 3.6: Point to Cell relation

Supposing that a particular CV does not change in time the time derivative of the conservative variables $\vec{W}$ can be cast in the form

$$\frac{\partial}{\partial t} \iiint_V \vec{W} dV = V \frac{\partial \vec{W}}{\partial t}$$

Therefore Equation (3.5) becomes

$$\frac{\partial \vec{W}}{\partial t} = -\frac{1}{V} \left[\oint_A \left(\vec{F}_c - \frac{1}{Re} \vec{F}_v \right) dA - \iiint_V \vec{Q} dV \right] \quad (3.12)$$

3.3.1 Spatial Discretisation

The surface integral on the right-hand side of Equation (3.12) is approximated by a sum of the fluxes crossing the faces of the CV. This approximation is called spatial discretisation. It is usually supposed that the flux is constant along the individual face and that it is evaluated at the midpoint of the face. The source term is generally assumed to be constant inside the control volume. However, in cases where the source term becomes dominant, it is advisable to evaluate $\vec{Q}$ as the weighted sum of values from the neighbouring control volumes. If we consider a particular cell's volume $V_{I,J,K}$, as displayed in Figure 3.3, we obtain from Equation (3.12)

$$\frac{\partial \vec{W}_{I,J,K}}{\partial t} = -\frac{1}{V_{I,J,K}} \left[\sum_{m=1}^{N_f} \left(\vec{F}_c - \frac{1}{Re} \vec{F}_v \right)_m \Delta A_m - \vec{Q}_{V_{I,J,K}} \right] \quad (3.13)$$

where N_f denotes the number of CV faces m (which is equal to 6 in 3D). The variable ΔA_m , stands for the area of the face m . For all CVs (I, J, K) a system of ordinary differential equations of first order are obtained which is hyperbolic in time, that means to advance them in time requires starting from a known initial condition ([67]). The indices in capital letters (I, J, K) reference the CV as shown in Figure 3.6. The term in the square brackets on the right-hand side of Equation (3.13) is also referred to as the *residual*. It is denoted by $\vec{R}_{I,J,K}$. Therefore Equation (3.13) can be simplified to

$$\frac{\partial \vec{W}_{I,J,K}}{\partial t} = -\frac{1}{V_{I,J,K}} \vec{R}_{I,J,K} \quad (3.14)$$

When the system of discretised governing equations (Equation (3.13)) is numerically solved, the flow variables with respect to the computational grid are stored at the cell centres. This strategy is called Cell-centred scheme, meaning control volumes are identical with the grid cells and the flow variables are associated with their centroids (see Figure 3.6). A wide range of choices exists with respect to the evaluation of the convective fluxes $\vec{F}_c$. The basic problem is that their values at all N_F faces of the control volume need to be known, but the flow variables are not directly available there. This means, either the fluxes or the flow variables need to be interpolated to the face of the control volume. This can in principle be achieved in two ways:

1. by arithmetic averaging like in central discretisation schemes (usually applied to convective term F_c);
2. by some biased interpolation like in upwind discretisation schemes, which take into account the characteristics of the flow (usually applied to diffusive term F_v).

The reason why the convective and diffusive fluxes are treated using different numerical methods is due to their mathematical nature. The viscous (diffusive) terms compose of smooth linear functions whereas the convective terms of nonlinear ones.

A schematic of the flux-cell value correspondence can be seen below in Figure 3.7.

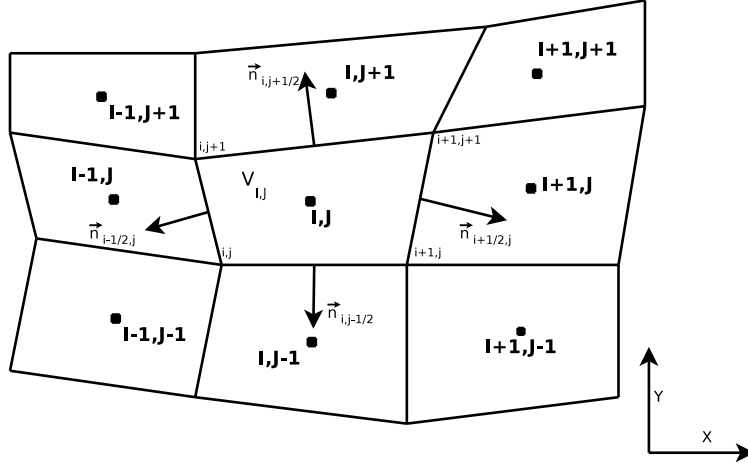


FIGURE 3.7: Fluxes and cell centre values

In the above schematic of Figure 3.7, the small indices relate to the cell points (or corners) and the capital indices to the cell centres as shown already in Figure 3.6.

In the case of arithmetic averaging, the task can be completed in two ways. Either by the *average of fluxes* (generally applied to the convective term) or the *average of variables*. Considering the average of fluxes to be computed for the convective flux $\vec{F}_c$ at cell face $\vec{n}_{i+\frac{1}{2},j}$ as shown in Figure 3.7 gives

$$\left(\vec{F}_c \Delta S\right)_{I+1/2,J} \approx \frac{1}{2} \left[\vec{F}_c \left(\vec{W}_{I,J}\right) + \vec{F}_c \left(\vec{W}_{I+1,J}\right) \right] \Delta S_{I+1/2,J} \quad (3.15)$$

On the other hand considering the average of variables the formulation will be

$$\left(\vec{F} \Delta S\right)_{I+1/2,J} \approx \vec{F} \left(\vec{W}_{I+1/2,J}\right) \Delta S_{I+1/2,J} \quad (3.16)$$

where the conservative (dependent) variables at the face $\vec{n}_{i+1/2,j}$ of the control volume are defined as the arithmetic average of values at the two adjacent cells.

$$\vec{W}_{I+1/2,J} = \frac{1}{2} \left(\vec{W}_{I,J} + \vec{W}_{I+1,J} \right) \quad (3.17)$$

Note that the flux vector $\vec{F}$ has no subscript and therefore could either be the inviscid or viscous flux vector.

The other case is to interpolate the flow quantities (those variables comprised in the vectors of Equation (2.13)) separately to both sides of the cell face. The interpolated

quantities, usually referred to throughout the literature as the *left* and *right state*, differ in general between both sides. The fluxes through the cell face are then evaluated by a non-linear function depending on the difference of the left and right state. This can be formulated in general as:

$$\left(\vec{F}_c \Delta A\right)_{I+1/2,J} \approx f_{Flux}\left(\vec{W}_L, \vec{W}_R, \Delta A_{I+1/2,J}\right) \quad (3.18)$$

where

$$\begin{aligned} \vec{W}_L &= f_{Interp}\left(\dots, \vec{W}_{I-1,J}, \vec{W}_{I,J}, \dots\right) \\ \vec{W}_R &= f_{Interp}\left(\dots, \vec{W}_{I,J}, \vec{W}_{I+1,J}, \dots\right) \end{aligned} \quad (3.19)$$

The same approximations can be extended very easily to a three dimensional case as that shown in Figure 3.3. So at the cell face $\vec{n}_{i+1/2,j,k}$ corresponding to $\vec{n}_2$ in Figure 3.3, Equation (3.17)-Equation (3.19) can be re-written as:

- *Average of*

Fluxes

$$\left(\vec{F}_c \Delta S\right)_{I+1/2,J,K} \approx \frac{1}{2} \left[\vec{F}_c\left(\vec{W}_{I,J,K}\right) + \vec{F}_c\left(\vec{W}_{I+1,J,K}\right) \right] \Delta S_{I+1/2,J,K} \quad (3.20)$$

Variables

$$\left(\vec{F} \Delta S\right)_{I+1/2,J,K} \approx \vec{F}\left(\vec{W}_{I+1/2,J,K}\right) \Delta S_{I+1/2,J,K} \quad (3.21)$$

$$\vec{W}_{I+1/2,J,K} = \frac{1}{2} \left(\vec{W}_{I,J,K} + \vec{W}_{I+1,J,K} \right) \quad (3.22)$$

- *Interpolation of Variables*

$$\left(\vec{F}_c \Delta A\right)_{I+1/2,J,K} \approx f_{Flux}\left(\vec{W}_L, \vec{W}_R, \Delta A_{I+1/2,J,K}\right) \quad (3.23)$$

where

$$\begin{aligned} \vec{W}_L &= f_{Interp}\left(\dots, \vec{W}_{I-1,J,K}, \vec{W}_{I,J,K}, \dots\right) \\ \vec{W}_R &= f_{Interp}\left(\dots, \vec{W}_{I,J,K}, \vec{W}_{I+1,J,K}, \dots\right) \end{aligned} \quad (3.24)$$

Note that in the method of variable interpolation the flux vector contains in this case a subscript, namely *c*, meaning that it is only applied to the convective flux vector. Further,

the left and right states are obtained by some function such as those presented later on in Section 3.4.2 and Section 4.1.1. The value at the face can then be calculated by using Flux Vector Splitting Methods (FVSM) or Flux Difference Splitting Methods (FDSM), see Riemann solvers in Section 4.1.2.

Concerning the last variable in Equation (2.13), that is the source term $\vec{Q}$, it is presumed that its value remains constant throughout the CV and for this very reason is calculated using the flow variables from the corresponding cell centre. Therefore it is defined as

$$\left(\vec{Q}V\right)_{I,J,K} = \vec{Q}\left(\vec{W}_{I,J,K}\right)V_{I,J,K} \quad (3.25)$$

Using the above relationships it is possible to compute numerically the fluxes through all the cell faces and accumulate them leading to the residual $\vec{R}_{I,J,K}$ in Equation (3.14).

3.3.2 Temporal Discretisation

It is reminded that the method of lines has been implemented thus allowing for a separate discretisation technique in space and in time if required. This offers a lot of freedom when considering different levels of approximation for the convective, diffusive and temporal derivatives. When the method of lines is applied to the governing equations it leads to the generalised form of Equation (3.14) as shown in Section 3.3.1. Note that it has been assumed that the grid is static, meaning that the volume of all the cells does not change with time and thus the volume variable V can be taken outside of the time derivative. It is now possible to approximate the time derivative by the following non-linear scheme ([70])

$$\frac{V}{\Delta t}\Delta\vec{W}^n = -\frac{\zeta}{1+\omega}\vec{R}^{n+1} - \frac{1-\zeta}{1+\omega}\vec{R}^n + \frac{V}{\Delta t}\frac{\omega}{1+\omega}\Delta\vec{W}^{n-1} \quad (3.26)$$

with

$$\Delta\vec{W}^n = \vec{W}^{n+1} - \vec{W}^n$$

being the solution correction. The superscripts $n+1$ and n denote the time levels where n is the current one and Δt represents the time step. Furthermore, the value the parameters ω and ζ take decide on the nature of the time-stepping method, that is whether it will be an explicit ($\zeta = 0$) or implicit scheme. Note however that due to the fact that the temporal and spatial discretisations are decoupled, attention has to be made when considering high resolution scheme methods such as TVD in which case it has to be satisfied individually for both temporal and spatial discretisations.

Explicit Type Runge-Kutta Time Integration

Explicit methods are characterised by the fact that the new value of the solution at time $n + 1$ can be **explicitly** expressed in terms of values obtained from previous timesteps $n < n + 1$ at the same control volume. Therefore in order to propagate the solution in time, an algebraic expression in terms of known previous solutions is only required to be evaluated. This makes explicit time-integration methods particularly simple to implement. The most basic time-integration scheme can be obtained by setting $\zeta = 0$ and $\omega = 0$ in Equation (3.26). This leads to the time derivative being approximated by a forward difference method, referred to as the first order in time forward Euler stepping, with the residual R evaluated at each successive current time level only as shown in Equation (3.27)

$$\vec{W}^{n+1} = \vec{W}^n - \frac{\Delta t}{V} \vec{R}^n \quad (3.27)$$

The forward Euler difference method represents a single-stage scheme as the new solution W^{n+1} is obtained from one evaluation of the residual. Very popular are multistage time-stepping schemes such as Runge-Kutta (RK) methods that evaluate the solution at the new timestep $n + 1$ by advancing it through a number of intermediate stages where at each one the residual is calculated. Coefficients are used to weigh the residual at each stage. Depending on the stage coefficients and number of stages, a multistage scheme can be extended to 2nd- or higher- order to accuracy. Further, the coefficients can be optimised in order to achieve a number of favourable conditions such as

- expand stability region [71, 72];
- improve damping properties for better convergence and robustness [73, 74, 75];
- preserve properties of the Total Variation Diminishing (TVD) and Essentially-Non-Oscillatory (ENO) spatial discretisation methods [76, 77].

A general form for the Runge-Kutta method advancing a solution from time level n to $n + 1$ by a timestep Δt through m stage(s) is given by [78]

$$\begin{aligned} \vec{W}_{I,J,K}^0 &= \vec{W}_{I,J,K}^n \\ \vec{W}_{I,J,K}^k &= \vec{W}_{I,J,K}^0 - \Delta t \sum_{j=0}^m \xi_{kj} R_{I,J,K}^j \\ \vec{W}_{I,J,K}^{n+1} &= \sum_{k=1}^m \xi_k R_{I,J,K}^k \end{aligned} \quad (3.28)$$

where k identifies the k -th Runge-Kutta stage ($k = 1, \dots, m$), ζ_{jk} and ξ_k are real numbers with ($j = 0, \dots, m$), yielding a truly explicit method provided $\zeta_{jk} = 0$ for $j \geq k$. The advantages which make explicit RK methods so widely adopted and used are the low cost per timestep computational effort as well as the relatively large stability region [78]. The order of accuracy of RK methods can be increased by arbitrarily increasing the number of stages m .

Timestep Calculation

A common value needed to be obtained for any numerical temporal discretisation is that of Δt . For an explicit time stepping scheme however it can be shown that the solution will remain stable only up to a certain maximum value of Δt . The restriction results from the local speed of the fastest wave s , propagating through a cell in the entire computational domain. A simple way to visualise this is by examining Figure 3.8.

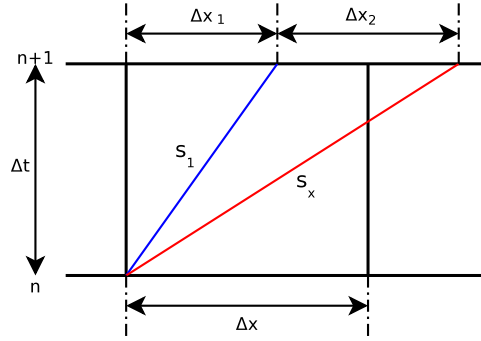


FIGURE 3.8: Fluxes and cell centre values

One can notice in Figure 3.8 that wave speed s_1 propagates for a timestep duration Δt within the cell domain (considering x-direction). Thus the solution obtained can be said to remain stable. However if a faster wave speed exists, such as s_x and within the same timestep length of Δt it 'escapes' the cell domain, then the solution is said to be unstable. For a time-stepping scheme to be stable it has to meet the **Courant-Friendrichs-Lewy** condition (CFL) which states that if a wave is crossing a discrete grid, then the timestep must be less than the time for the wave to travel adjacent grid points. As a corollary, when the grid point separation is reduced, the upper limit for the time step also decreases. As will be seen later this has the effect of reducing the time step to a very small amount when dealing with solid surfaces leading to considerable computational time requirements. From Figure 3.8 it is derived that the maximum timestep length for a one dimensional linear

hyperbolic set of partial differential equations solved on a structured orthogonal grid can be given by:

$$\Delta t = \frac{\Delta x}{\max(s)} \quad (3.29)$$

The above relationship Figure 3.29 can be further extended to the full 3D non-linear NSE for a structured grid to:

$$\Delta t = \min \left(C \frac{V_{I,J,K}}{\max(|s_i^j|)_{I,J,K}} \right) \quad (3.30)$$

where $i = 1, \dots, 5$ represents the five possible characteristics of Equation (2.13) that s can take and $j = \{(x, y, z) \vec{n}\}$ is the face's projected length to the axial direction considered. Also, the extension of a one dimensional formulation to a three dimensional domain by 'sweeping' through each three dimensions using the same one-dimensional equations is referred to as directional splitting. Further, a new coefficient is introduced, C , denoting the CFL number. The CFL number takes positive values between zero and one and its actual purpose is to further control the value of Δt in order to maintain stability. Note that it is introduced due to the non-linear nature of the governing equations in which case it is possible for a wave to vary in a non-linear manner and therefore reach the adjacent grid point within the time calculated by the assumed linear wave.

3.4 Upwind Methods

In hyperbolic problems such as the set of equations in Equation (2.13), information is propagated in waves moving along characteristics which are lines in the flow along which the value of the characteristic variable does not change. For a system of equations, several waves propagating at different speeds and directions are possible. Thus it makes sense to try and use the knowledge of the structure of the solution to determine more accurate and *physically correct* flux functions. This idea led to the rise of *upwind* methods in which the information for each characteristic variable is obtained depending on the direction of the waves as seen in Figure 3.9 below. Note that upwind methods are used for the spatial discretisation of the convective terms in the hyperbolic NSE.

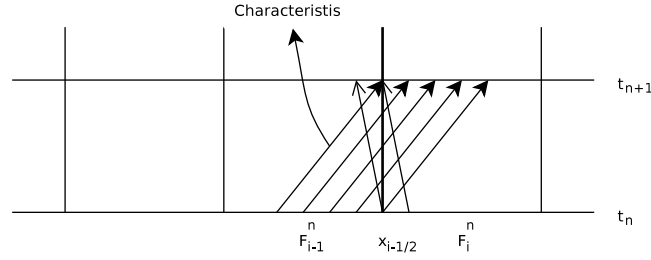


FIGURE 3.9: Upwind wave propagation and direction

Considering the full 3D NSE as in Equation (2.13) it is derived that there is a total of six directions, two for each axis, and a total of five characteristic variables originating from the convective flux [79]. Note that the diffusive flux also has five characteristics but are not dealt with since it's linear nature does not require a rigorous numerical treatment in order for it's solution to be obtained. Naturally as can be seen in Figure 3.9, upwind methods generate a left and right value of the flowfield variables for a cell face resulting in a similar system to that of a classical fluid mechanic problem, the shock tube problem. The first to notice this similarity and though to extend it to the NSE to solve the non-linear Euler equations was Godunov [80].

3.4.1 Shock Tube and Riemann Problem

A shock tube is a closed tube initially divided into two sections separated by a fixed diaphragm, one with a high pressure p_H and the other with a low pressure p_L as can be seen in Figure 3.10(a) and the fluid remaining at rest. If the diaphragm is instantly removed, then the high pressure gradient will cause a shock wave travelling to the right, an isentropic expansion wave propagating to the left and a contact surface separating the two different fluids emerging due to the different process they underwent as seen in Figure 3.10(b). The main noticeable difference in the two resulting fluids emerges from the fact that the shock wave will cause a change in enthalpy whereas the isentropic expansion will not thus resulting in a contact surface where the two fluids meet.

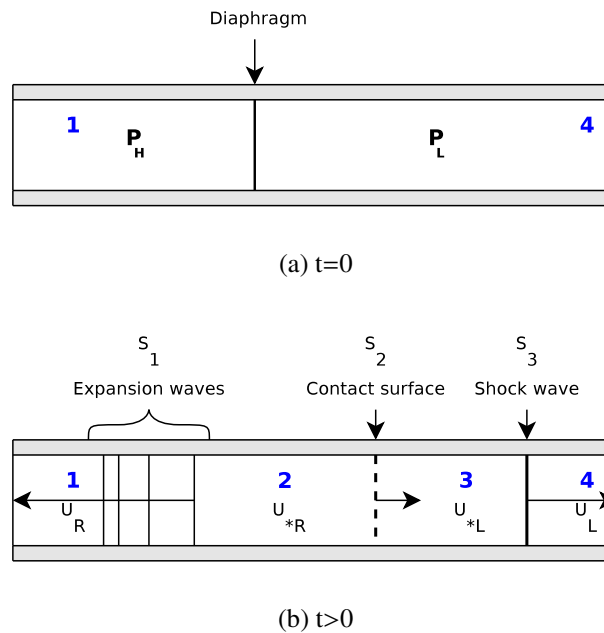


FIGURE 3.10: Shock tube

The solution of the flowfield in the shock tube as sketched in Figure 3.10 is referred to as the *Riemann problem*, named after the German mathematician G.F. Bernhard Riemann who first attempted its solution in 1858, and is a direct analytic solution of the unsteady, one-dimensional Euler equations. Briefly, the solution method developed is based on a few principles. First, all the properties of regions 1 and 4 are known before the diaphragm is removed and remain the same in the regions where the shock or the expansion waves have yet to pass after a given time from the diaphragm removal. A set of equations can be used to estimate the values past the expansion waves, however an initial estimate and iterative procedure is required in order to solve the set of equations to obtain the flowfield variables past the shock.

3.4.2 Application to Finite Volume Method - Godunov's Method

As already mentioned, a hyperbolic method with a set of equations contains more than one wave and direction. Thus it is possible that there may be waves travelling in both directions, so an upwind method will still have to consider information from both sides when estimating the characteristic variable. This is typically done by using characteristic decomposition often via the solution of the Riemann problem as presented in 3.4.1. The

paths which the waves follow as a function of time can be seen in Figure 3.11. The first to suggest such a method was S.K. Godunov ([80]) who based his idea on the shock tube problem as previously mentioned.

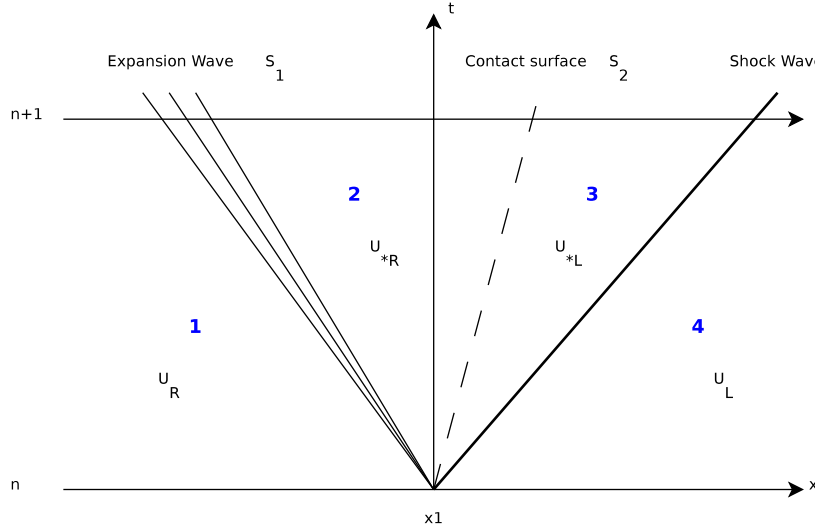


FIGURE 3.11: Wave diagram

This clearly reflects a similar problem faced in the shock tube problem above in Section 3.4.1. Put in the FVM context it can reflect the different characteristics of the flow-field structure situated to the left and right of a CV's face. This can be clearly seen in Figure 3.12. Note that regions 1 and 4 in Figure 3.11 correspond to the values obtained for the left and right state of the cell's face and the in between regions 2 and 3 correspond to the equal number fluid states of Figure 3.10.

However there is a difference in the application of the Riemann solver to FVM. The position, existence and direction of either wave, that be shock wave or rarefaction, can vary meaning that any combination of shock wave and rarefaction is possible for the left and right waves as well as whether the direction is to the left or right. For example it could be possible that there are no rarefactions and instead there are two shock waves, one either side of the contact surface wave but all propagating to the same direction. This would leave the variable values at the face to be equal to those on the opposite side.

Further, it is possible that the characteristic do not follow a straight line as depicted in Figure 3.11 for which case the only correct solution is to use an exact Riemann solver. However this requires a time consuming and computer resource 'hungry' iterative procedure for which linearised and/or approximate Riemann solvers have been developed

instead (see Section 4.1.2).

The purpose of solving the Riemann problem is to determine the value of the upwind flux of each variable at the cell face. This can be achieved by using the exact Riemann solver but for the reasons just mentioned alternate methods have been developed. One method approximates the exact Riemann problem and estimates in which of the states (regions) the cell face will be after a finite timestep (ie HLL(C) Riemann solver) for which the flux can be analytically obtained. Alternatively, the exact solution of a linearised (approximate) Riemann problem can be used to calculate the net flux contribution of each individual wave according to it's strength and characteristic speed (Roe's [81] and CBS method [82] use *characteristic decomposition*) to estimate the total interface variable flux.

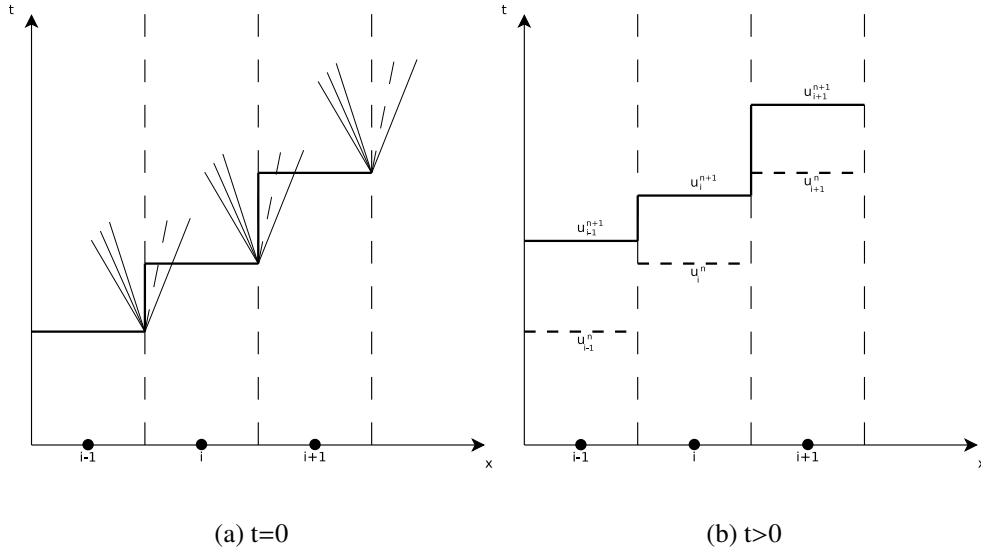


FIGURE 3.12: Shock tube application to cell centred FVM

Common to any of the above approaches is the requirement for a left and right value of the flowfield variables to the cell face. In Godunov's original method the flowfield variable values for the right and left state to the cell face are taken equal to the values at the cell centre of the corresponding side. Therefore Godunov's method uses a piecewise constant function to interpolate the cell centre values to the cell face as seen in Figure 3.12(b) and for this reason is considered a first order accurate method. The formulation of the

piecewise constant function when applied to Equation (3.24) is as:

$$\begin{aligned} \left(\vec{F} \Delta A \right)_{I+1/2,J,K} &= \text{Riemann} \left(\vec{W}_L, \vec{W}_R, \Delta A_{I+1/2,J,K} \right) \\ \vec{W}_L &= \vec{W}_{I,J,K} \\ \vec{W}_R &= \vec{W}_{I+1,J,K} \end{aligned} \quad (3.31)$$

To obtain better accuracy the cell centre values must be interpolated to the cell's face in a different manner than just piecewise constant. One simple way of achieving this would be to allow the piecewise constant function have a non-zero slope thus leading to a piecewise linear function. These different reconstruction methods form the basis of *high resolution* methods which are considered next.

3.4.3 High Resolution Methods

Within upwind methods a certain type of methods called *High Resolution Methods* are included. As already stated, first order reconstruction techniques are able to capture the position of discontinuities in the flow, such as shock waves, accurately but introduce a very large amount of artificial dissipation resulting in smeared results for discontinuities and poor turbulent results in the smooth regions of the flow. On the other hand second order reconstruction techniques are much less dissipative in smooth regions of the flow but tend to introduce unphysical oscillations near discontinuities.

The purpose of high resolution methods is to manage to maintain the second order's of accuracy non-dissipative nature in the smooth regions of the flow while switching to the first order near discontinuities. This leads to a general definition for high resolution methods which defines them as

‘methods that select the most appropriate technique for approximating the solution given the nature of the flow provided by the local solution’

Naturally, Godunov's method is regarded as a high resolution method, the first to be developed. It uses a piecewise constant interpolation to obtain the cell face values from the cell centre values and is therefore considered a first order method. As a results of Godunov's method, it emerged that no linear method can be both second-(or higher) order and monotone. This obstacle led to the development of modern high resolution methods.

High-resolution methods were developed in order to circumvent Godunov's theorem [80] which states:

'There are no monotone, linear schemes for the linear advection equation of second or higher order of accuracy'

High-resolution methods achieve this by using non-linear differencing. A number of different high-resolution methods for solving the convective fluxes F_c in Equation (3.13) are available. No matter the method though, the result of the application of a high resolution method must meet all of the following requirements in order for it to be considered successful according to Harten's definition [83]:

- Provide at least second order of accuracy in smooth areas of the flow.
- Produce numerical solutions (relatively) free from spurious oscillations.
- In the case of discontinuities, the number of grid points in the transition zone containing the shock wave is smaller in comparison with that of first-order monotone methods.

The various schemes available for solving the convective flux are briefly described later on in Section 4 as developed in [84, 85, 86].

Should be noted that these methods are nonlinear in nature even if the equation being solved are linear. The nonlinearity is introduced through the reconstruction of the flow-field variable values by adapting them according to the character of the local solution. In the case of high resolution methods of non piecewise constant interpolation, the question of the slope of the variable reconstruction from the cell centre to the cell face naturally arises. The slope is effected by the reconstruction method and is what leads second order methods generate oscillations near discontinuities.

The desired goal in a high resolution method is to maintain the second order of accuracy while guaranteeing that no nonphysical oscillations occur. This is achieved by incorporating a number of restrictions to the desired numerical methods which will allow it to comply to certain rules. Such rules are monotonicity preserving, total variation and monotone which are discussed next.

Monotonicity Preserving

A scheme is called monotonicity preserving if

$$W_I^n \geq W_{I+1}^n \quad \text{for all } i \quad (3.32)$$

leads to

$$W_I^{n+1} \geq W_{I+1}^{n+1} \quad \text{for all } i \quad (3.33)$$

A simple graphical example can be seen below in Figure 3.13. If the function varies according to the relationship of Equation (3.32), then it can be visualised as the graph in Figure 3.13(a). Otherwise it could take the shape of Figure 3.13(b). Hence if a scheme is monotonicity preserving, the propagation of a discontinuity may lead to it becoming smeared in future time steps but not oscillatory.

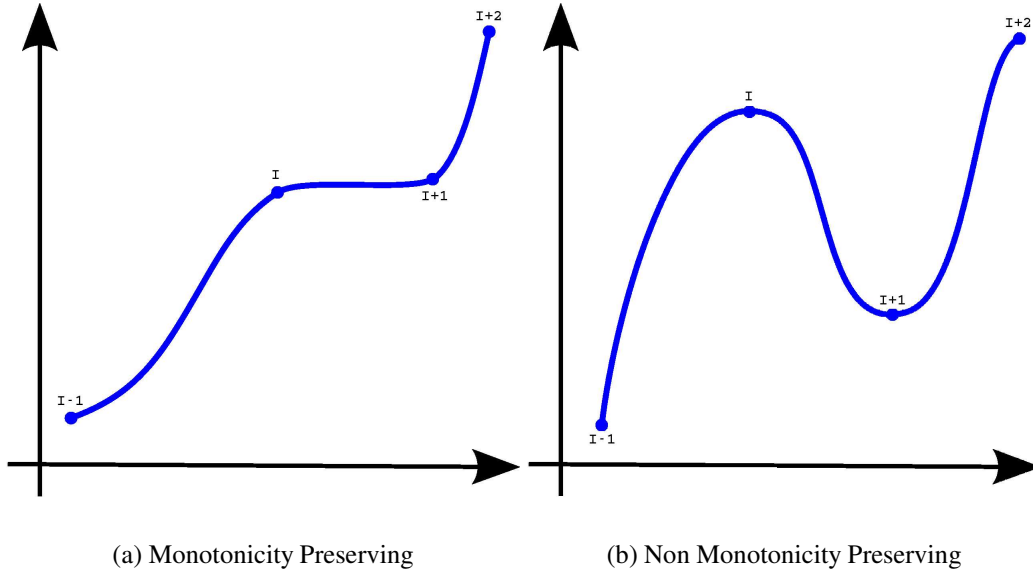


FIGURE 3.13: Plots of a 1-Dimensional function distribution

Total Variation Diminishing

Total Variation Diminishing (TVD) methods are developed based on the notion of the *total variation* of the flowfield variable oscillations in the solution. Considering just the one-dimensional in space direction x of variable array $\vec{W}$, thus becomes $W_i(x)$, has a total variation defined by:

$$TV(\vec{W}) = \limsup_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \int_{-\infty}^{+\infty} |W(x + \epsilon) - W(x)| dx \quad (3.34)$$

When considering the full NSE then the $\vec{W}$ is also dependent on time, $W(x, t)$, in which case the total variation is defined at a fixed time t . In a discretised domain, like that

of a FVM, $\vec{W}$ is a function of the mesh and its total variation at a time instant t at iteration level n is given by:

$$TV(W^n) = \sum_{i=-\infty}^{+\infty} |W_{i+1}^n - W_i^n| \quad (3.35)$$

where function $W(x, t)$ is assumed to reach a zero or constant value as it reaches the infinity boundaries in order to obtain a finite total variation. A scheme is regarded as a TVD method when the following constraint is met:

$$TV(W^{n+1}) \leq TV(W^n) \quad (3.36)$$

The above relationship in Equation (3.36) is built on the principle that the true (physical) solution to the advection equation propagates at a speed u with unchanged shape, so that the total variation $TV(W(x, t))$ remains constant in time. However a numerical method may produce results that do not adhere to the constant total variation. In that case the total variation of $\vec{W}$ may increase with time, leading to the spurious oscillations. By a method satisfying Equation (3.36), it can avoid generating unphysical oscillations. Note that any TVD method is also monotonicity preserving.

Monotone Methods

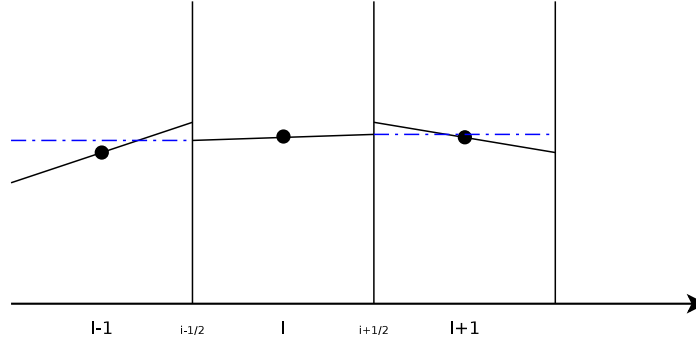
The monotonicity property is physically inherent to the flowfield and to which any numerical method, such as a high resolution method, must abide too. In order for a numerical method to sustain the *monotonicity property* the following conditions must be met [83]:

- No new local extrema in $\{x, y, z\}$ may be created;
- The value of a local minimum increases, i.e., it is a non-decreasing function and the value of a local maximum decreases, i.e., it is a non-increasing function

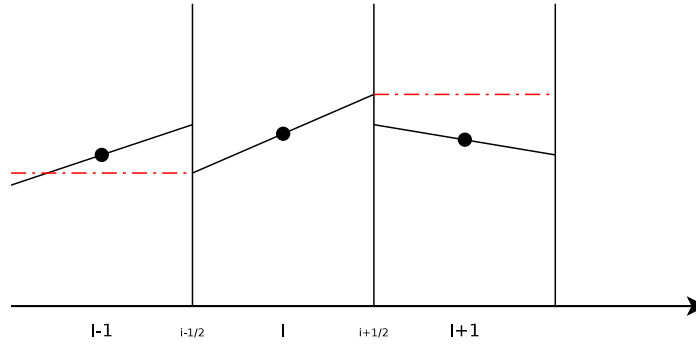
These can be satisfied by the above two restrictions, that is monotonicity preserving and TVD. When applied to a numerical method, monotonicity preserving ensures a given monotone initial condition remains monotone. This is also ensured by TVD but further extended to a non monotone initial condition for which it does not ensure a monotone solution but ensures the non monotone 'error' does not increase. Therefore an additional law can be introduced to enable a scheme become inherently monotone. By observing the monotone variation of a function such as in Figure 3.13(a) one can deduct that a scheme

will be monotone if the ratio between successive gradients remains lower than one, that is for x-direction W_x

$$\frac{W_{I+1} - W_I}{W_I - W_{I-1}} \leq 1 \quad (3.37)$$



(a) Monotone



(b) Non Monotone

FIGURE 3.14: Geometric representation of monotone vs. non monotone limiter

This is applied numerically to the code through the reconstruction stage and can be visualised as in Figure 3.14 from which it is evident that the reconstructed value at a cell face must remain within the range of values of it's left and right cell centre values, so

$$W_I \leq W_{i+1/2} \leq W_{I+1} \quad (3.38)$$

Monotonicity preserving is the weakest of the three conditions mentioned. This implies that if a numerical method is monotone, it is also TVD. Further, if a method is TVD

then it is also monotonicity preserving but it is not necessarily monotone. The stated relationships can be mathematically expressed as

$$S_{MP} \supseteq S_{TVD} \supseteq S_M \quad (3.39)$$

where S_{MP} stands for monotonicity preserving schemes, S_{TVD} for TVD schemes and S_M for monotone schemes.

4

Numerical Methods

In this chapter more details on the numerical methods employed to solve the NSEs are given. Specifically a detailed description of the numerical methods used to solve the discretised form of the NSEs (see Chapter 3) are presented.

The ability of the method of lines to use different discretised methods for the temporal and spacial discretisation is taken advantage of. Thus the temporal NSEs components are treated by using explicit two and three stage Runge-Kutta (RK) methods within the LES context. The solution of the spatial components of the NSEs employ Godunov-like methods. No source terms apart from the forcing term presented in Section 5 are required for the simulated cases and therefore will be ignored henceforth. Both feature very modern numerical methods developed recently such as high resolution and TVD schemes and are applicable on a structured grid composing of quadrilateral (2D) or hexahedra (3D) elements, whether single or multi-grid, single block or multi-block.

Furthermore the discretisation of the spatial components of the NSEs, those being the convective and diffusive terms, are treated using different methods where the viscous terms are centrally discretised and the convective are discretised using various high-resolution methods.

The interpolation is carried out in the reconstruction stage which is considered as the first part of the spatial discretisation of the convective term. In the second part of this first stage, the Riemann solver is used to obtain the flux at the cell face. For this purpose, the exact or approximate Riemann solvers is widely used. The fluxes obtained from the spatial reconstruction is used as the input to the Riemann solver. It allows superior wave capturing and improves the numerical modelling of smooth and non smooth waves. The flux is then accumulated at all faces over a CV along with the viscous fluxes which are obtained by central differences. As the second step, solution progresses from time step n to $n + 1$ via a RK timestepping method.

Note that in the formulation of the methods, directional splitting has been employed meaning that the theory obtained for a one dimensional problem is extended to a three dimensional problem by applying the one dimensional relationships separately but similarly for each of the three dimensions.

4.1 Convective Term

As already mentioned in Section 3, the convective flux is obtained in two stages, firstly being the reconstruction phase which is then followed by the solution of the Riemann problem. Both parts are presented next.

4.1.1 Reconstruction

In this section, the formulae used in order to obtain the interpolated cell face flowfield variable values as discussed in Section 3.3.1 and formulated for a three dimensional case in Figure 3.24 are presented. The basis of any high resolution method is to first obtain the left and right values to be applied to the Riemann problem. These left and right values are obtained at a cell face by some interpolation function using the existing cell centre flowfield variable solution at the current time level.

A popular approach of achieving this is to formulate the interpolated left and right states using the Monotone Upstream-Centred Schemes for Conservation Laws (MUSCL) method with further utilisation of slope limiters ([87]). Otherwise, it is possible to also achieve this by using the Weighted Essentially Non-Oscillatory (WENO) scheme as proposed by [88].

MUSCL Schemes

The left and right states of the conservative variables W at cell interface $i+1/2$ are computed according to [79] as

$$\begin{aligned} W_{i+1/2,j,k}^L &= W_{I,J,K} + \frac{1}{4} \left[(1-k) \phi(r^L) \Delta W_{I,J,K}^- + (1+k) \phi\left(\frac{1}{r^L}\right) \Delta W_{I,J,K}^+ \right] \\ W_{i+1/2,j,k}^R &= W_{I+1,J,K} + \frac{1}{4} \left[(1-k) \phi(r^R) \Delta W_{I+1,J,K}^+ + (1+k) \phi\left(\frac{1}{r^R}\right) \Delta W_{I+1,J,K}^- \right] \end{aligned} \quad (4.1)$$

where

$$r^L = \frac{\Delta W_{I+\frac{1}{2},J,K}}{\Delta W_{I-\frac{1}{2},J,K}}, \quad r^R = \frac{\Delta W_{I+\frac{1}{2},J,K}}{\Delta W_{I+\frac{3}{2},J,K}} \quad (4.2)$$

further

$$\begin{aligned} \Delta W_{I+\frac{1}{2},J,K} &= W_{I+1,J,K} - W_{I,J,K}, \quad \Delta W_{I-\frac{1}{2},J,K} = W_{I,J,K} - W_{I-1,J,K}, \\ \Delta W_{I+\frac{3}{2},J,K} &= W_{I+2,J,K} - W_{I+1,J,K} \end{aligned} \quad (4.3)$$

Note that $\phi(r)$ is the slope limiter function used to 'correct' the reconstructed value to one satisfying either of the monotonicity preserving, TVD or monotone laws. Finally the parameter k is used to determine the spatial accuracy of the interpolation. In this case a value of $k = \frac{1}{3}$ is used, resulting in a three point interpolation formula which constitutes (in the FVM framework [78]) a second order upwind biased scheme.

It has to be mentioned that the original MUSCL scheme developed by Van Leer [89, 90, 91, 92, 93] was designed to 'mix' a first order scheme (Godunov's piecewise constant reconstruction) with a second order scheme. The idea was that the most suitable of the methods would be used according to the local slope, i.e. if a sharp discontinuity was detected the first order scheme would be used otherwise for smooth regions a second order scheme would be used instead. Note that the first order scheme is always monotone, something that does not mean that the second order scheme would also be. In fact it could be possible that the second order scheme would not even meet the requirement of monotonicity preserving let alone monotone. The consequence of this was still the generation of oscillations near discontinuities though to a much lesser degree as opposed to just using the second order scheme as is.

Thus the slope limiter function was introduced into the formulation of the MUSCL

scheme in order for the second order scheme to become either monotonicity preserving, TVD or monotone according to it's numerical design. Most slope limiters developed for second order schemes are shown to be TVD compliant [94]. Among the second order limiters used are namely Van Leer's limiter (VA limiter) and Monotonized Central difference limiter (MC limiter) which was also proposed by Van Leer [92]. Further, a more recent, fifth order reconstruction (5th order MUSCL limiter) within the MUSCL framework [95, 96] has also been introduced. The formulae to obtain the slopes $\phi(r)$ of each of the above mentioned limiters is given by

Second Order A variety of CFD textbooks include and present in detail a number of second order limiters because of their popularity and wide spread use in the CFD community. Some of the aforementioned have slopes given by

VL limiter

$$\phi_{VL}(r) = \frac{r + |r|}{1 + |r|}$$

MC limiter

$$\phi_{MC}(r) = \max\left(0, \min\left(\frac{1+r}{2}, 2, 2r\right)\right)$$

Fifth Order A fifth order MUSCL scheme was recently developed in [95, 96] and is given by:

$$\begin{aligned}\phi_{M5}(r^L) &= \max\left(0, \min\left(2, 2r_i^L, \varphi^L\right)\right) \\ \phi_{M5}(r^R) &= \max\left(0, \min\left(2, 2r_{i+1}^R, \varphi^R\right)\right)\end{aligned}\quad (4.4)$$

where

$$\varphi^L = \frac{-2/r_{i-1}^L + 11 + 24r_i^L - 3r_i^L r_{i+1}^L}{30}, \quad \varphi^R = \frac{-2/r_{i+2}^R + 11 + 24r_{i+1}^R - 3r_{i+1}^R r_i^R}{30} \quad (4.5)$$

Due to the larger stencil required for fifth order accuracy, the number of total slopes required has obviously increased too, defined as

$$\begin{aligned}r_{i-1}^L &= \frac{\Delta W_{I-\frac{1}{2},J,K}}{\Delta W_{I-\frac{3}{2},J,K}}, & r_i^L &= \frac{\Delta W_{I+\frac{1}{2},J,K}}{\Delta W_{I-\frac{1}{2},J,K}}, \\ r_{i+1}^L &= \frac{\Delta W_{I+\frac{3}{2},J,K}}{\Delta W_{I+\frac{1}{2},J,K}}\end{aligned}\quad (4.6)$$

and

$$\begin{aligned} r_{i+2}^R &= \frac{\Delta W_{I+\frac{3}{2},J,K}}{\Delta W_{I+\frac{5}{2},J,K}}, & r_{i+1}^R &= \frac{\Delta W_{I+\frac{1}{2},J,K}}{\Delta W_{I+\frac{3}{2},J,K}}, \\ r_i^R &= \frac{\Delta W_{I-\frac{1}{2},J,K}}{\Delta W_{I+\frac{1}{2},J,K}} \end{aligned} \quad (4.7)$$

WENO Schemes

WENO schemes are a recent method of reconstruction '*built*' on top of the Essentially Non-Oscillatory (ENO) concept originally proposed by [76, 97]. The difference between ENO and MUSCL schemes is the way each one deals with the slopes that are obtained. In MUSCL, limiters are used in order to control the slope of the higher than one order schemes to avoid the generation of oscillations near discontinuities. ENO schemes employ a different philosophy to achieve this while still managing to obtain a higher than one order of accuracy. It achieves this by simply choosing the smoothest of all the slopes obtained in its stencil, be that second or even higher order method.

A recent improvement of ENO schemes is WENO primarily based on the work done in [88, 98, 99]. As the name implies, WENO schemes are *weigh* each slope based on some criteria (such as smoothness following ENO schemes) and uses the slope obtained by the combination of all the slopes obtained, depending on the order of the method, instead of employing just the smoothest one. This results in a convexly weighted average of polynomial interpolated slopes according to the smoothness of each slope. Because of considering all slopes calculated, WENO schemes can reach higher orders of accuracy than ENO methods, which on the contrary achieve lower orders of accuracy since they discard most of them.

In order to obtain the polynomial $\pi_{I,J,K}(x)$, cell centre values of each CV is used to obtain values at the cell face. After the interpolated polynomials are combined to give a new polynomial $\Pi_{I,J,K}(x)$. Considering a face at $i + 1/2$ with cell centre values at I and $I + 1$ to the left and right respectively and a third order WENO reconstruction using linear interpolation gives the following polynomials:

$$\begin{aligned} \pi_L(x) &= W_{I,J,K} + \frac{\Delta W_{i-1/2}}{\Delta x_{i-1/2}} (x - x_i) \\ \pi_R(x) &= W_{I,J,K} + \frac{\Delta W_{i+1/2}}{\Delta x_{i+1/2}} (x - x_i) \end{aligned}$$

The calculation of the weighted average polynomial $\Pi(x)$ of the above polynomials yields the reconstructed variables at the cell faces left and right of each cell centre I and $I + 1$, i.e. for I the following reconstructions $(W_R)_{i-1/2}$ and $(W_L)_{i+1/2}$ are obtained. The convex combination is defined by

$$\Pi(x) = \frac{a_L}{a_L + a_R \pi_L(x)} + \frac{a_R}{a_L + a_R \pi_R(x)} \quad (4.8)$$

with

$$a_L = \frac{C_L}{IS_L^2}, \quad a_R = \frac{C_R}{IS_R^2} \quad (4.9)$$

where C_L and C_R are optimal weights and IS_L and IS_R are smoothness indicators given by

$$IS_L = \left(\Delta W_{i-1/2,j,k} \right)^2, \quad IS_R = \left(\Delta W_{i+1/2,j,k} \right)^2 \quad (4.10)$$

Naturally, as the order of reconstruction increases, so does the number of stencils (cell centres) required to be taken into account too; in smooth regions, accuracy may be as high as $N/2 - 1$, where N being the number of samples. The derivation of a higher-order method follows along the same line, though as one would expect, the complexity of the equations rises with an increasing order of accuracy, see [83, 98, 99] for more details.

4.1.2 Riemann Solver

As mentioned in Section 3.4, the Riemann problem is used to compute the flux through all the faces of a CV given a value for either side of the face. However solving the Riemann problem exactly is not always necessary and due to its numerical and thus also computationally demanding requirements, approximate Riemann solvers are used instead. One of the most popular approximate Riemann solvers is the Harten, Leer, Lax Contact (HLLC) Riemann solver [79, 85, 100] which is an extension of the Harten, Leer, Lax (HLL) Riemann solver [101] by taking into consideration the existence of the contact surface. Many other approximate Riemann solvers exist such as Osher's Riemann solver [102, 103], Roe's Riemann solver [104] and the Characteristic Based (Riemann) Solver (CBS) [85]. From these the HLLC and CBS Riemann solver were selected.

HLLC

In this method, to determine the numerical fluxes, the speed of the five waves has to be estimated initially. Note that from [79] it is known that the characteristic speed waves $c_{2,3,4}$ are equal (meaning $c_2 = c_3 = c_4$) and thus from now on the Riemann problem will be approximated by a three wave structure as shown in Figure 3.11. Note also that the following nomenclature is considered

$$S_L = c_1, \quad S_R = c_5, \quad S_\star = c_{2,\dots,4} \quad (4.11)$$

The methodology used to obtain the wave (characteristic) speed estimates for $S_{L,\star,R}$ as shown in Figure 3.11 is based on a pressure-velocity coupling as detailed in [79, 85] by the following formulae

$$S_L = v_L - \alpha_L q_L, \quad S_\star = u_\star, \quad S_R = v_R + \alpha_R q_R \quad (4.12)$$

where

$$q_K = \begin{cases} 1 & \text{if } p_\star \leq p_K \\ \left[1 + \frac{\gamma+1}{2\gamma} (p_\star/p_K - 1)\right]^{1/2} & \text{if } p_\star > p_K \end{cases} \quad K = R \text{ or } K = L \quad (4.13)$$

The wave relations used are exact but the pressure ratio across a shock is approximated. The pressure in the star region $p_\star$ is thus obtained by [105]

$$p_\star = \frac{1}{2} (p_L + p_R) - \frac{1}{2} (v_R - v_L) \bar{\rho} \bar{\alpha} \quad (4.14)$$

where $\bar{\rho}$ and $\bar{\alpha}$ are the local mean values given by

$$\bar{\rho} = \frac{1}{2} (\rho_L + \rho_R), \quad \bar{\alpha} = \frac{1}{2} (\alpha_L + \alpha_R) \quad (4.15)$$

and the characteristic speed $u_\star$ in the star region is then given by

$$u_\star = \frac{1}{2} (W_L - W_R) - \frac{1}{2} \frac{(p_R - p_L)}{\bar{\rho} \bar{\alpha}} \quad (4.16)$$

Last parameter required is the speed of the characteristic in the star region $S_\star$. This can be obtained by

$$S_\star = \frac{p_R - p_L + \rho_L \vee_L (S_L - \vee_L) - \rho_R \vee_R (S_R - \vee_R)}{\rho_L (S_L - \vee_L) - \rho_R (S_R - \vee_R)} \quad (4.17)$$

Finally, the flux F_c for the HLLC approximate Riemann solver is then given by

$$(F_c)_{i+\frac{1}{2}}^{HLLC} = \begin{cases} (F_c)_L & \text{if } 0 \leq S_L, \\ (F_c)_{*L} & \text{if } S_L \leq 0 \leq S_\star, \\ (F_c)_{*R} & \text{if } S_\star \leq 0 \leq S_R, \\ (F_c)_L & \text{if } S_R \leq 0, \end{cases} \quad (4.18)$$

CBS

The Characteristic Based Scheme (CBS) is a linearised Riemann Solvers. It was first developed and presented in [106] for the compressible Euler equations and extended further by [9, 107]. It defines the conservative variables along the characteristics as functions of their characteristic values. A recent derivation of the scheme can also be found in [108] and results in the following linear system to compute the flux

The cell $W_{i-1/2,j,k}$ can now be calculated using the CBS Riemann solver by the following relation:

$$W_{i-1/2,j,k} = \begin{pmatrix} \rho \\ (\rho u) \\ (\rho v) \\ (\rho w) \\ \rho E \end{pmatrix} = \begin{pmatrix} \rho_0 + r_1 + r_2 \\ (\rho u)_0 + (u + \alpha) r_1 + (u - \alpha) r_2 \\ (\rho v)_0 + v r_1 + v r_2 \\ (\rho w)_0 + w r_1 + w r_2 \\ (\rho u)_0 + (H + \alpha c_0) r_1 + (H - \alpha c_0) r_2 \end{pmatrix} \quad (4.19)$$

where r_1 , r_2 and H (total enthalpy) are given by:

$$r_1 = \frac{1}{2\alpha^2} \left\{ (\rho_0 - \rho_1) \left(\alpha c_0 - \frac{\hat{\gamma}}{2} y^2 \right) + [(\rho u)_0 - (\rho u)_1] (\hat{\gamma} u - \alpha) + \right. \\ \left. [(\rho v)_0 - (\rho v)_1] \hat{\gamma} v + [(\rho w)_0 - (\rho w)_1] \hat{\gamma} w - (e_0 - e_1) \hat{\gamma} \right\} \quad (4.20)$$

$$r_1 = \frac{1}{2\alpha^2} \left\{ -(\rho_0 - \rho_2) \left(\alpha c_0 - \frac{\hat{\gamma}}{2} y^2 \right) + [(\rho u)_0 - (\rho u)_2] (\hat{\gamma} u - \alpha) + \right. \\ \left. [(\rho v)_0 - (\rho v)_2] \hat{\gamma} v + [(\rho w)_0 - (\rho w)_2] \hat{\gamma} w - (e_0 - e_2) \hat{\gamma} \right\} \quad (4.21)$$

$$H = \frac{\alpha^2}{\hat{\gamma}} + 0.5y^2 \quad (4.22)$$

The values of the velocities u , v , w and α (speed of sound) are the average of their left and right states while $y^2 = u^2 + v^2 + w^2$ and $\hat{\gamma} = \gamma - 1$. The advective flux $(F_c)_{i-1/2}$ for the CBS is calculated by:

$$(F_c)_{i-1/2}^{CB} = F(W_{i-1/2}) \quad (4.23)$$

4.2 Diffusive Term

The discretisation of the viscous flux F_v of the NSE (Equation (2.16)) is done as already mentioned by the method of *average of variables* (see Section 3.3.1) and formulated for a two and three dimensional case as Equation (3.16) and 3.21 respectively. When applying the average of variables method to the viscous flux for a three dimensional case while considering the i -index direction, it is given by

$$(F_v)_{i+1/2,j,k} = \frac{1}{2} \left((F_v)_{I,J,K} + (F_v)_{I+1,J,K} \right) \quad (4.24)$$

The remaining task is the calculation of the velocity derivatives in order to compute the stress tensor $\bar{\bar{\tau}}$ (see Equation (2.10)) and the temperature derivatives (see Equation (2.17) in Section 2.4). A common numerical method employed here is to use *Gauss' theorem*, however other methods also exist such as applying *finite differences* or *Green's theorem* in case of two dimensions. The CV used here for the calculation of the viscous flux F_v is generally the same as that utilised in the calculation of the convective fluxes in order to obtain a consistent spatial discretisation. However the fact that velocity and temperature derivatives have to also be obtained at each cell face's midpoint, requires the construction of an additional CV for their estimation. The constructed Auxiliary CV (referred to as AuxCV from now on) has the following properties:

- AuxCV's cell centre is located at the CV's face midpoint under consideration;
- AuxCV's cell corners are located at the midpoints of each CV's cell edge.

A schematic of the above while considering the i -index (x-axis direction) can be clearly seen in Figure 4.1 below.

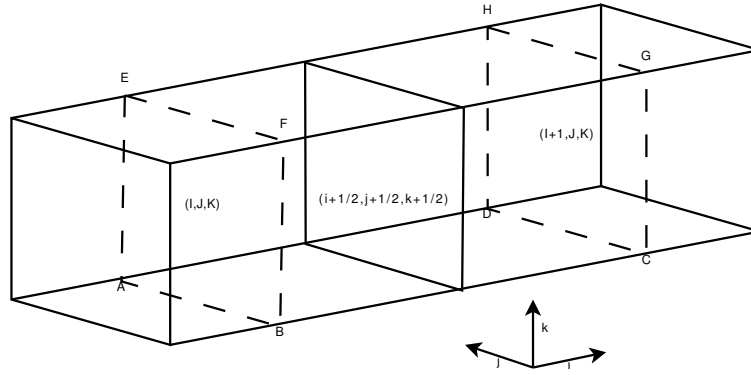


FIGURE 4.1: Dual control volume schematic

The new AuxCV is bounded in Figure 4.1 by the lettered corners $A-H$. The logical counters for the corner points are given in Table 4.1 below

TABLE 4.1: Index notation for auxiliary control volume's corners

A:	i	$j-1/2$	$k-1/2$
B:	i	$j-1/2$	$k+1/2$
C:	$i+1/2$	$j-1/2$	$k+1/2$
D:	$i+1/2$	$j-1/2$	$k-1/2$
E:	i	$j+1/2$	$k-1/2$
F:	i	$j+1/2$	$k+1/2$
G:	$i+1/2$	$j+1/2$	$k+1/2$
H:	$i+1/2$	$j+1/2$	$k-1/2$

The location of the corner points is determined by arithmetic averaging, i.e. the x -coordinate of point A is given by

$$x_{i,j+1/2,k+1/2} = \frac{1}{2} \left(x_{i-1/2,j+1/2,k+1/2} + x_{i+1/2,j+1/2,k+1/2} \right)$$

Using Gauss' theorem (see Equation (A.2) in Appendix A.1.4), an estimate for the average value of the velocity (or temperature) gradient can be obtained as a function of the boundary values of a control volume. Hence for an arbitrary volume V enclosed by a boundary surface A with a variable field $\vec{u}$, Gauss' theorem gives

$$\iiint_V (\nabla \cdot \vec{u}) dV = \oiint_A \vec{u} \cdot d\mathbf{A} \quad (4.25)$$

and discretising for an AuxCV of volume V'

$$\begin{aligned} (\nabla \cdot \vec{u}) V' &= \sum_{m=1}^{N_f} \bar{u}_m \cdot \vec{n}_m S'_m \Rightarrow \\ \nabla \cdot \vec{u} &= \frac{1}{V'} \sum_{m=1}^{N_f} \bar{v}_m S'_m \end{aligned} \quad (4.26)$$

where $\bar{v}_m$ is the average value of the contravariant velocity on the m^{th} surface of the cell, and the summation is over the number of faces N_f of AuxCV. Note that in for a hexahedron cell, N_f is equal to six, that is $N_f = 6$. Further, the surface area S'_m and volume V' of the auxiliary CV (AuxCV) are calculated the same way as done for the CV in Section 3.2. Also the midpoint cell face values of the derivative components such as velocity $\bar{v}_m$ for the AuxCV are taken equal to the cell centre values of the CV.

Once the values for the flow variables and of the first derivatives are obtained at the faces of the CV, their contribution to the viscous flux can be summed according to Equation (2.16)-2.17. In turn the viscous flux is placed into Equation (3.13) with the convective flux calculated earlier completing the spatial discretisation, leaving the time integration to be computed next.

4.3 Time Marching

The solution of the unsteady NSE requires a numerical method in order to march the solution in time. In the present frame all computations were carried out using a three-stage TVD ([77],[85]) embedded explicit Runge-Kutta (RK) time marching method. When combined with a TVD spatial discretisation method as well, it has been shown that it can produce results that comply with TVD but at the cost of more function evaluations.

The methods were developed in [77] with the resulting three stage method expressed mathematically as

$$\begin{aligned} W^1 &= W^n + \frac{\Delta t \vec{R}^n}{V} \\ W^2 &= \frac{3}{4}W^n + \frac{1}{4}W^1 + \frac{1}{4} \frac{\Delta t \vec{R}^1}{V} \\ W^{n+1} &= \frac{1}{3}W^n + \frac{2}{3}W^2 + \frac{2}{3} \frac{\Delta t \vec{R}^2}{V} \end{aligned} \quad (4.27)$$

4.3.1 Global Timestep Computation

As shown in Section 3.3.2, Δt is the global timestep used in all the cells, for which given a Courant-Friedrichs-Levy (CFL) number, it is obtained by Equation (3.30) for the three dimensional NSE. More analytically it is given by

$$\Delta t = \min \left[CFL \frac{V}{\max (|c_l^x|, |c_l^y|, |c_l^z|)} \right] \quad (4.28)$$

where V denotes the cell volume computed by Equation (3.11), $\vec{c}_l^{x,y,z}$ are the characteristic speeds in each direction (x, y, z) and ($l = 0, \dots, 5$) are the number of characteristics of the compressible NSE as formulated in Equation (2.13).

4.4 Low Mach Number Treatment

The standard MUSCL extrapolation has been augmented using the method of [109], which ensures uniform dissipation of kinetic energy in the limit of zero Mach number (M). The theoretical development and justification of the method can be further found in [110]. This modification extends the validity of the Godunov method to at least $M \approx 10^{-4}$, via a progressive central differencing of the velocity components, without changing the formulation of the underlying governing equations or sacrificing monotonicity of the density field.

It was shown in [109] that the leading order kinetic energy dissipation rate is proportional to $u^3/\Delta x$, similar in form to that proposed by [5] for decaying turbulence. It is this dissipation rate which acts as a subgrid model in the ILES framework, giving significantly improved high wavenumber performance compared to standard Godunov methods

([109]). It should be noted that in the literature so far, there has been no case in which the LMNT has been applied to an inhomogeneous anisotropic turbulent flow with no-slip wall boundary condition. The Low Mach Number Treatment (LMNT) works by '*correcting*' the left and right values obtained from the reconstruction in such a way that, as the local Mach number progressively decreases, they will not introduce any further dissipation. This is achieved by the following formulae as introduced in [109]:

$$\vec{u}_{i+1/2,j,k}^R = \frac{\vec{u}^L + \vec{u}^R}{2} + z \frac{\vec{u}^L - \vec{u}^R}{2}, \quad \vec{u}_{i+1/2,j,k}^L = \frac{\vec{u}^L + \vec{u}^R}{2} + z \frac{\vec{u}^L - \vec{u}^R}{2} \quad (4.29)$$

where z is defined as

$$z = \min(M_{total}, 1) \quad , \quad M_{total} = \max(M_L, M_R) \quad (4.30)$$

and M_L is the local Mach number to the left of the cell face and M_R similarly but to the right. This approach is shown [109, 110] to be a simple solution to the problem of excessive *numerical* dissipation by modifying the velocity '*jump*' at the cell interface by a function z . The method ensures that the dissipation does not exceed that of the original scheme and reverts to the standard upwind form in supersonic flows. At the same time it can be considered as a '*realistic*' physical law addition to the standard Godunov method because of the new treatment of the velocity jumps, which otherwise Godunov's method would set up artificially large jumps not really present in a low Mach number flowfield. Further, it can be seen as a progressive central differencing of the velocity components as Mach number tends to zero.

As probably noticed, the reconstructed left and right density and pressure are not modified, but since the velocity flux has altered, the total energy flux will need to be corrected to accommodate for the new kinetic energy (KE) flux as according to Equation (2.3). It is important to point out that the reconstruction is modified based on the local properties of the flowfield, hence the same governing equations are solved throughout the domain and thus it's additional computational '*effort*' is considerably small.

Simulated Cases and Results

5

Channel Flow

5.1 Introduction

Channel flow is regarded as a fundamental topic for research on turbulence. The fact that there are only two straight and parallel plates alone means that the reasons for the existence and sustainability of turbulence will clearly depend on the Reynolds number, that is the properties of the flow and also the computer algorithm used. Also, most engineering applications, deal with wall bounded or at least solid walls and is therefore of great importance to model correctly and accurately. Thus it is an excellent case to use to investigate a CFD algorithm's ability in modelling turbulence in the presence of a solid surface. It is regarded [34] as a complementary case to the homogeneous decaying turbulence in a triply periodic cube since an inhomogeneous direction is added due to the presence of the no-slip wall resulting in a fully developed anisotropic inhomogeneous flow. Thus the ability of modelling and capturing a turbulent boundary layer is investigated.

5.2 Problem Description

As already mentioned the channel flow configuration consists of two flat and parallel plates at a distance H between them. The size of the channel in this case is $2\pi \times 2 \times \pi$ in length (L), height (H) and spanwise width (W) that is in the x , y and z axis correspondingly. In the streamwise and spanwise direction a periodic boundary condition is used and a no-slip (wall) condition along the surfaces of the plates. A diagram of the problem depicting the above can be seen below in Figure 5.1 and 5.2.

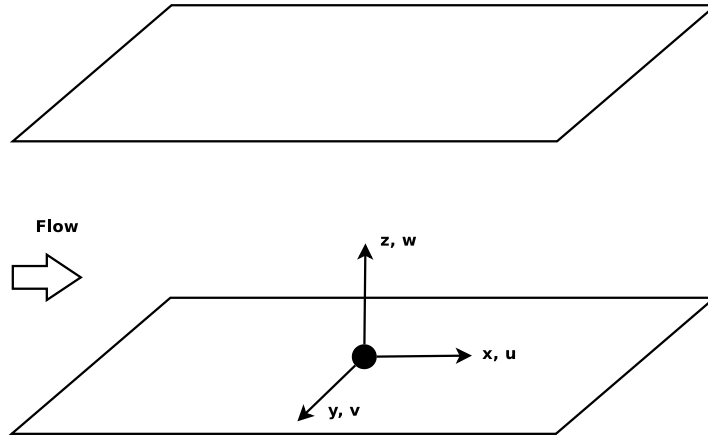


FIGURE 5.1: Coordinate system in channel

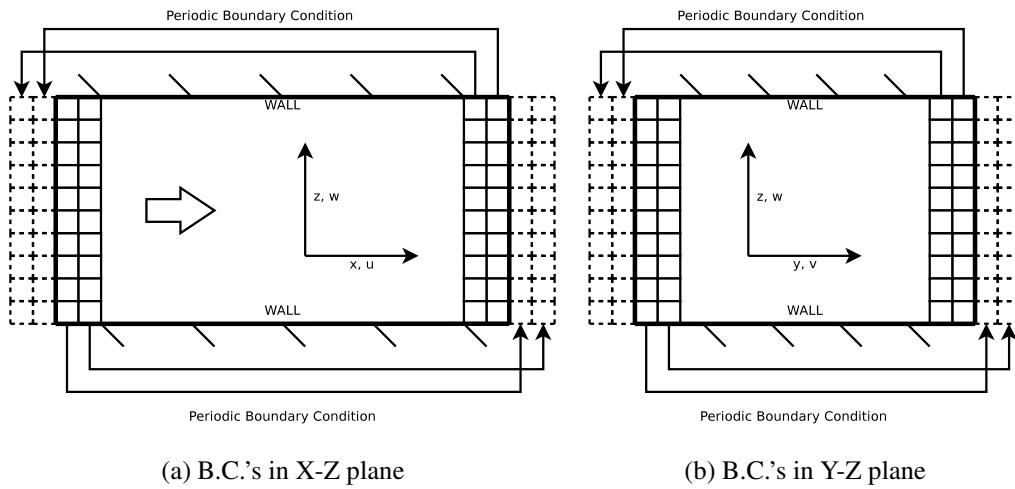


FIGURE 5.2: Boundary conditions used

The flow modelled is air at standard atmospheric ground level conditions. Three Reynold's numbers based on friction velocity are investigated in [35], equal to $Re_\tau = 180$, $Re_\tau = 395$ and $Re_\tau = 590$. From these the $Re_\tau = 395$ was chosen to conduct all simulations and which is later converted to the Reynolds number based on mean flow velocity. The results obtained from the ILES code used in this thesis (referred to as CNS3D from now on) will be compared against those from DNS [35]. Note that there is no experimental computation conducted in the selected Reynolds number however there do exist others relatively close. In [45], the experiments were conducted using different Reynolds numbers from which the closest one to 395 was at $Re_\tau \approx 424$ and in [44] at $Re_\tau \approx 335$.

5.3 Methodology

This section examines initially the theory behind any of the newly applied methods and explains in detail how any changes and/or additions were implemented to the CNS3D code.

5.3.1 Theory

Reynolds Number

It is common practise in journals concerning channel flow configurations to give the Reynolds number based on the wall shear velocity u_τ , that is to provide the wall shear Reynolds number Re_τ . But it is also usefull to know the Reynolds number based on the mean velocity Re_m . To achieve this the following is done:

- From [111], it is possible to relate the wall shear Reynolds number with the Reynolds number based on the bulk velocity:

$$\begin{aligned} Re_\tau &= 0.09 Re_m^{0.88} \Rightarrow \\ Re_m &= \left(\frac{Re_\tau}{0.09} \right)^{1/0.88} \end{aligned} \quad (5.1)$$

Hence the Reynolds number based on the bulk velocity is computed. Note that since the code does not use the friction flow parameters as given in DNS [35] for non-dimensionalisation, the Reynolds number must be based on the reference values.

From non-dimensionalisation it follows that $Re_c = Re_m$ and the above formulae of Equation (5.1) is used to convert Re_τ to Re_m . Thus the values of Re_τ obtained from CNS3D will be obtained depending on the code's ability to model turbulence in the near wall region.

- It is also known from [111] that:

$$Re_0 = \frac{3}{4} Re_m \quad (5.2)$$

Keep in mind that Re_0 is based on the centreline velocity and thus it is sometimes unclear if it is based on the centreline velocity of a laminar flow (parabolic profile) or that of a fully developed turbulent flow. In DNS is it custom to give the latter.

- It is also important to keep in mind the following definitions:

$$\begin{aligned} Re_\tau &= \frac{u_\tau \delta}{\nu} \\ Re_m &= \frac{U_m(2\delta)}{\nu} \\ Re_0 &= \frac{U_0 \delta}{\nu} \end{aligned} \quad (5.3)$$

, where

$$u_\tau = \langle \mu \rangle_z \left. \frac{\partial \langle u_z \rangle}{\partial z} \right|_{z=0}$$

5.3.2 Initial Conditions

The initial condition for the simulation is similar to that used in [52]. The streamwise velocity is given a laminar parabolic profile perturbed with random noise ε which is generated in Fortran 77 code through the RAND intrinsic function. For the spanwise and wall-normal velocity components, the local streamwise value is used but multiplied by a different random noise signal and by a perturbation magnitude percent.

$$\begin{aligned} \rho(t=0) &= 1 \\ u(t=0, z) &= U_0 \left[1 - (z-1)^2 \right] (1 + s\varepsilon) \\ v(t=0, z) &= s\varepsilon \times u(t=0, z) \\ w(t=0, z) &= s\varepsilon \times u(t=0, z) \\ E(t=0, z) &= \frac{P}{\gamma-1} + \frac{\rho}{2} (u^2 + v^2 + w^2) \end{aligned} \quad (5.4)$$

, where U_0 is the centreline velocity, P is the pressure, s is the percent of perturbation and ε is a random number $\varepsilon \in [-1, 1]$. Note that,

$$U_0 = \frac{3}{2}U_m$$

known from [111]. An example of the resulting profiles can be seen below in Figure 5.3-5.5. The streamwise non-dimensional velocity $\frac{u}{U_m}$ is

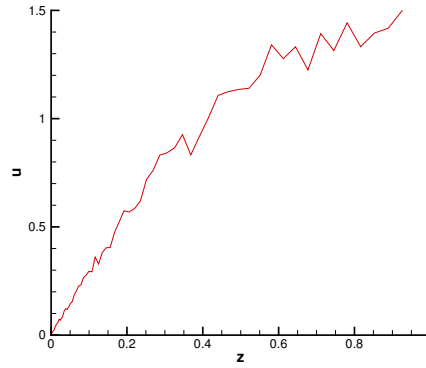
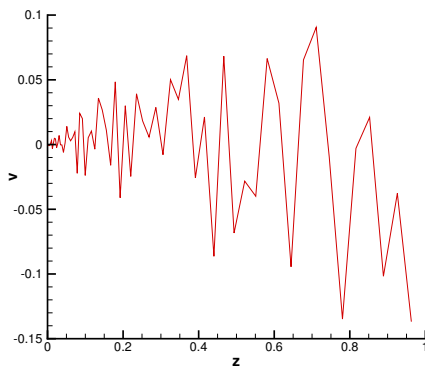
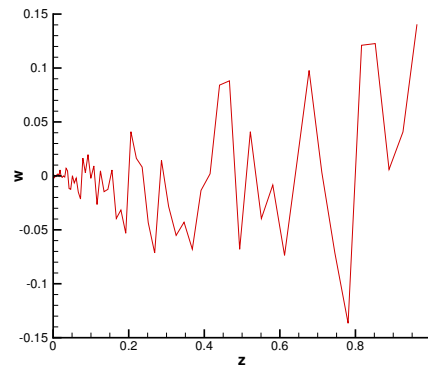


FIGURE 5.3: Initial u-velocity

whereas the spanwise velocity $\frac{v}{U_m}$ and wall normal velocity $\frac{w}{U_m}$ are



(a) Initial v-velocity



(b) Initial w-velocity

FIGURE 5.4: Initial Conditions Used in X-Z plane

and the total energy E

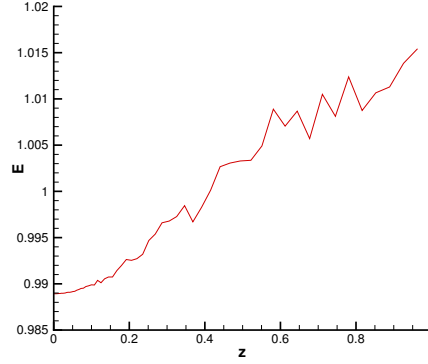


FIGURE 5.5: Initial total energy E

Note that density is given just a constant value of $\frac{\rho}{\rho_c} = 1$ since the flow to be simulated is in the incompressible regime of the Mach number ($M < 0.3$) and can be considered nondimensionally as equal to one.

Three different initial conditions were investigated. The only difference between each case was the magnitude of the perturbation parameter ε . The values considered were 0%, 10% and 30%. The reason for conducting this investigation was first to justify using any form of perturbation in the flow in the first place and secondly to see if the difference in the initial perturbation magnitude would have an effect on the turbulence intensities obtained later on once the flow had developed to a turbulent state, that is if at all. It was found that having a larger initial perturbation magnitude helped in the flow developing slightly faster, however no difference was made in the obtained friction Reynolds number once both 10% and 30% cases fully develop. Further, for 0% perturbation the flow did not become turbulent at all within the numerical study's timeframe, though it may be possible at a much later time. For numerical stability reasons the 10% perturbation will be used in all subsequent simulations to be presented.

5.3.3 Mass Flux Preservation

Two ways have been developed and used in literature to deal with preserving the mass flux. One achieves mass-flux preservation by 'tweaking' the periodic boundary condition and the other by adding an additional 'artificial' streamwise pressure derivative term to the NSE. Both these methods were implemented and compared to a case where no massflux

preserving condition was enforced in order to justify the need for applying any method in the first place.

Mass-Flux Preserving Periodic Boundary Condition

Since the flow is unsteady, the mass flow rate will fluctuate. The new boundary condition is a modified periodic boundary condition. It is similar to the periodic boundary condition meaning that it mirrors all the variables but it is different in that the mirrored values of the streamwise velocity are 'corrected' such that the mass flow rate across the inlet and outlet achieves a target value.

The formulae used at the inlet and outlet boundary conditions are:

$$U_{inlet} = \beta_f U_{outlet}$$

where,

$$\beta_f = \frac{Q_{target}}{Q_{outlet}}$$

where,

$$Q_{outlet} = \int_{z_{min}}^{z_{max}} \int_{y_{min}}^{y_{max}} [U(x_{outlet}, y, z) \delta y \delta z] dy dz$$

and

$$Q_{target} = U_m \times (y_{max} - y_{min}) (z_{max} - z_{min})$$

The same procedure is followed to correct the values of streamwise momentum copied from the inlet to the outlet ghost cells.

Forcing Term

In this case the streamwise pressure gradient in the NSE is accompanied by an 'artificial' forcing term. This is used to maintain the correct mass flux and since it is included in the NSE it means that it effects the whole domain and not just a part of it as in the previous massflux preserving periodic boundary condition method. This method was first used for compressible flow calculations in [55, 112] and is basically an additional numerical parameter (source term) that mimics the streamwise pressure gradient in order to maintain a pressure drop that satisfies the required massflux condition. Below are the modified streamwise momentum and energy equations of the NSE incorporating the forcing term

and using the summation convention for the repeated indices:

$$\begin{aligned} \frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) + \frac{\partial p}{\partial x_i} + f_i \delta_{il} &= \frac{\partial \sigma_{ij}}{\partial x_j} \\ \frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j} (E + p) u_j + f_i u_i &= \frac{\partial}{\partial x_j} (\sigma_{ij} u_i) - \frac{\partial}{\partial x_j} q_j \end{aligned} \quad (5.5)$$

, where t and x_i are the independent variables representing time and spatial co-ordinates respectively, f_i is the forcing term, σ_{ij} is the viscous stress tensor, δ_{ij} is the Kronecker symbol defined as $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ otherwise and q_j is the heat flux. The equation to calculate the forcing term f_i is derived by the following steps:

1. Averaging the momentum equation over xy planes and integrating the result in the wall-normal direction, obtains:

$$\frac{\partial}{\partial t} Q_m = \frac{1}{Re} L_y \left[\langle \mu \rangle_{xy} \frac{\partial \langle u_1 \rangle}{\partial z} \right]_{z=0}^2 - L_y L_z f_1$$

, where the $\langle \rangle_{xy}$ operator stands for averaging over the xy plane, L_z is the width of the channel (wall normal), L_y its span and Q_m is the mean flux of the flow across a yz plane.

2. As long as

$$\langle \mu \rangle_{xy} \frac{\partial \langle u_1 \rangle}{\partial z} \bigg|_{z=2} = - \langle \mu \rangle_{xy} \frac{\partial \langle u_1 \rangle}{\partial z} \bigg|_{z=0}$$

, one gets

$$\frac{\partial}{\partial t} Q_m = -L_y L_z f_1 - 2 \frac{1}{Re} L_y \langle \mu \rangle_{xy} \frac{\partial \langle u_1 \rangle}{\partial z} \bigg|_{z=0}$$

This equation shows that if a constant forcing term f_1 is imposed, while the flow undergoes a transition leading to an increase of the shear stress

$$\langle \mu \rangle_{xy} \frac{\partial \langle u_1 \rangle}{\partial z} \bigg|_{z=0}$$

, the mass flux will decrease. So, if a constant mass flux ($\partial Q_m / \partial t = 0$) is desired, the driving term f_1 must be time-dependent for a fully developed turbulent flow (unsteady flow).

3. An extension of the procedure to compressible flows was done in [113] and is used

to compute the forcing term at each time step:

$$f_1^{n+1} = f_1^n + \frac{\Delta t}{L_y L_z} \left[\alpha (Q^{n+1} - Q_0) + \beta (Q^n - Q_0) \right] \quad (5.6)$$

, where Q_0 , Q^n and Q^{n+1} are , respectively, the mass flux (what is trying to be conserved), the mass flux at time step n and a first-order predictor of the mass flux at time step $n + 1$, given by

$$Q^{n+1} = Q^n - \Delta t g^n \quad (5.7)$$

, with

$$g^n = L_y L_z f^n + \frac{2L_y}{Re} \langle \mu^n \rangle_{xy} \left. \frac{\partial \langle u_1^n \rangle}{\partial z} \right|_{z=0} \quad (5.8)$$

Note that the forcing term in a steady flow simulation would eventually converge to a constant value, whereas for an unsteady simulation it will fluctuate around a mean value once the flow has been fully developed.

5.3.4 Time Averaging, Mean Flow Properties Calculation

Should be noted that the timestep duration changes at each timestep since it needs to be recalculated for the newly obtained solution. It is adaptive and therefore every timestep will have a different weighting in the averaging conducted. There are two possible approaches to average, one is using the timestep duration and the other is using the total run time. By using time in the averaging, instead of the iteration numbers, it is possible to take into account the variation in duration of every individual timestep. A general equation in calculating the mean of a variable ψ in time is

$$\bar{\psi}(t) = \frac{1}{t_{start} - t_{end}} \int_{t_{start}}^{t_{end}} \psi dt$$

and is used to obtain the mean values shown later in it's discretised form:

$$\bar{\psi}^{N+1} = \bar{\psi}^N \frac{T_{total}^N}{T_{total}^{N+1}} + \psi^{N+1} \frac{T_{current}^{N+1}}{T_{total}^{N+1}}$$

5.3.5 Important equations

In this section the superscript (*) sign referring to the nondimensional counterpart of a variable is again adopted in order to derive the nondimensional equations required to compute necessary flow parameters. The following is done in order to calculate the wall shear stress:

$$\tau_w = \mu \left(\frac{\partial u}{\partial y} \right) \Big|_{y=0} = \mu^* \left(\frac{\partial u^*}{\partial y^*} \right) \Big|_{y=0} \frac{\mu_c u_c}{l_c} \Rightarrow$$

$$\frac{\tau_w}{\frac{\mu_c u_c}{l_c}} = \mu^* \left(\frac{\partial u^*}{\partial y^*} \right) \Big|_{y=0} \Leftrightarrow \tau_w^* = \mu^* \left(\frac{\partial u^*}{\partial y^*} \right) \Big|_{y=0}$$

For the calculation of the shear velocity:

$$u_\tau = \sqrt{\frac{\tau_w}{\rho}} \Rightarrow u_\tau^2 = \frac{\tau_w}{\rho} = \frac{\tau_w^*}{\rho^*} \frac{\mu_c u_c}{\rho_c} = \frac{\tau_w^*}{\rho^*} \frac{\mu_c u_c}{\rho_c l_c} \Rightarrow$$

$$u_\tau^2 = \frac{\tau_w^*}{\rho^*} \frac{\mu_c u_c}{\rho_c l_c} = \frac{\tau_w^*}{\rho^*} \frac{\mu_c}{u_c \rho_c l_c} u_c^2 \Rightarrow \frac{u_\tau^2}{u_c^2} = \frac{\tau_w^*}{\rho^*} \frac{\mu_c}{u_c \rho_c l_c} \Rightarrow$$

$$\frac{u_\tau^2}{u_c^2} = \frac{\tau_w^*}{\rho^*} \frac{\mu_c}{u_c \rho_c l_c} \Rightarrow u_\tau^* = \sqrt{\frac{\tau_w^*}{\rho^*} \frac{1}{Re_c}}$$

The friction Reynolds number is calculated by the following formula:

$$Re_\tau = \frac{\rho u_\tau \delta}{\mu} = \frac{\rho_c u_c l_c}{\mu_c} \frac{\rho^* u_\tau^* \delta^*}{\mu^*} = Re_c \frac{u_\tau^*}{\mu^*}$$

From now on the (*) symbol is omitted and nondimensional units are insinuated.

5.3.6 High order statistics

The following statistics have also been implemented:

- Variable Profiles ψ ;
- Reynolds Stresses $(\psi' \psi')$;
- Skewness (S_ψ) ;
- Flatness (F_ψ) .

In order to calculate the Reynolds stresses, the fluctuating component of the variable needs to be calculated (ψ'). This is done by using the formula:

$$\psi' = \psi - \bar{\psi}$$

, where ψ is an unsteady variable. The dash (') denotes the fluctuating part of the variable whereas the overbar ($\bar{}$) denotes the mean. Note that since the conservative form of the NSE is used, that is momentum $\rho \mathbf{v}$ is calculated, and the compressible solver can lead to variations in density ρ , the velocity $\mathbf{v}$ needs to be decoupled from density ρ in order to compare velocity profiles with those obtained by the incompressible DNS [35]. This is done by using Favre averaging on the mean and the formulation holds as:

$$\bar{\psi} = \frac{\langle \rho \psi \rangle_{xy}}{\langle \rho \rangle_{xy}} \quad (5.9)$$

where $\langle \rangle_{xy}$ stands for the variable space average in the xy plane, where x is the stream-wise, y is the spanwise and z is the wall normal direction also referred to as ensemble averaging. Favre averaging is sometimes used in compressible flow to separate turbulent fluctuations from the mean-flow.

Once the fluctuating velocity field is obtained, it is possible to compute the Root Mean Square (RMS) profiles as well as all of the rest of the statistics mentioned above. The formula used for this purpose is as follows:

$$\psi_{rms}|_{z=0}^{z_{max}} = \left. \langle \sqrt{\psi'^2} \rangle_{xy} \right|_{z=0}^{z_{max}}$$

where $|_{z=0}^{z_{max}=2}$ stands for the variables profile in the z-axis. The Reynolds stresses computed use the velocity fluctuation fields. The general formula used to obtain each velocity component's Reynolds stress is as follows:

$$Re(\psi\psi)|_{z=0}^{z_{max}} = \left. \frac{\langle \psi'\psi' \rangle_{xy}}{u_\tau^2} \right|_{z=0}^{z_{max}}$$

The skewness and flatness are considered as higher order statistics and their statistical convergence is a good indicator that the flow has fully developed. The skewness is given by the following formula:

$$S_{\psi'} = \left. \frac{\langle \psi'^3 \rangle_{xy}}{\sqrt[3]{\langle \psi'^2 \rangle_{xy}}} \right|_{z=0}^{z_{max}}$$

, whereas the flatness by:

$$F_{\psi'} = \frac{\langle \psi'^4 \rangle_{xy} \Big|_{z=0}^{z_{max}}}{\langle \psi'^2 \rangle_{xy}^2 \Big|_{z=0}^{z_{max}}}$$

Skewness and flatness factors of velocity are important statistical properties that represent characteristics of turbulence. The production of the rate of dissipation of turbulent kinetic energy, or equivalently, the production of enstrophy is directly related to skewness in isotropic turbulence [114].

5.3.7 Grid clustering

The equation used to cluster the points near the wall uses the hyperbolic tangent equations and is taken from [115]. If $L(z)$ is the length at a given point number z and z_{start} and z_{end} are the start and end lengths, then an appropriate normalised length variable would be:

$$L^*(z) = \frac{L(z) - z_{end}}{z_{start} - z_{end}}$$

so that $0 \leq L^*(z) \leq 1$ as $z_{start} \leq L(z) \leq z_{end}$. The tangential stretching function used then is:

$$s = P \times L^*(z) + (1 - P) \left\{ 1 - \frac{\tanh [Q (1 - L^*(z))]}{\tanh (Q)} \right\}$$

, where P and Q are parameters to provide grid point control. P effectively provides the slope of the distribution, $P \times L^*(z)$, close to $L^*(z) \approx 0$. Q is called a damping factor and control the departure from the linear s versus $L^*(z)$ behaviour. Small values of Q cause small departures from linearity. However, if P is close to unity the departure from linearity will be small and will occur only for $L^*(z)$ close to unity. Once s is obtained it is used to specify the distribution of $L(z)$ as follows:

$$L(z) = z_{end} + (1 - s)(z_{start} - z_{end})$$

The grids sizes used can be seen in Table 5.1 below:

TABLE 5.1: Grids along with properties

Grid	Domain Size ($L_x \times L_y \times L_z$)	Grid Size ($N_x \times N_y \times N_z$)	$\Delta z(z^+)$
Grid 1	$2\pi\delta \times 2\delta \times \pi\delta$	$64 \times 48 \times 68$	0.003 (1.185)
Grid 2	$2\pi\delta \times 2\delta \times \pi\delta$	$96 \times 96 \times 96$	0.00253205 (1.00016)
Grid 3	$2\pi\delta \times 2\delta \times \pi\delta$	$128 \times 128 \times 128$	0.00188365 (0.74404)
DNS[35]	$2\pi\delta \times 2\delta \times \pi\delta$	$256 \times 192 \times 193$	0.000075298 (0.03)

A clear comparison between the different grid point numbers, cell sizes and clustering employed in the wall normal direction can be seen in Figure 5.6 below

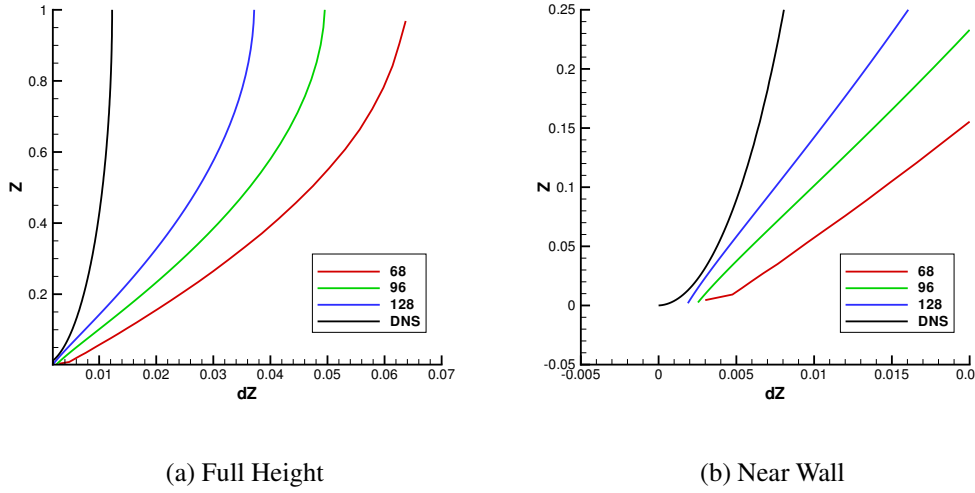


FIGURE 5.6: Wall normal clustering of all grids

In the above graph (Figure 5.6(a)), the individual wall normal length (or cell height) can be seen, thus depicting the clustering of each grid employed for easy comparison. However, the most important region is the wall region. There, apart from the fact that the smallest turbulent scales exist, a boundary layer is also present because of the combination of the solid wall and the viscous flow considered and therefore introduces an additional parameter that the grid needs to be able to capture. Because of this importance an additional graph similar to Figure 5.6(a) but focused closer to the wall is shown along with it Figure 5.6(b).

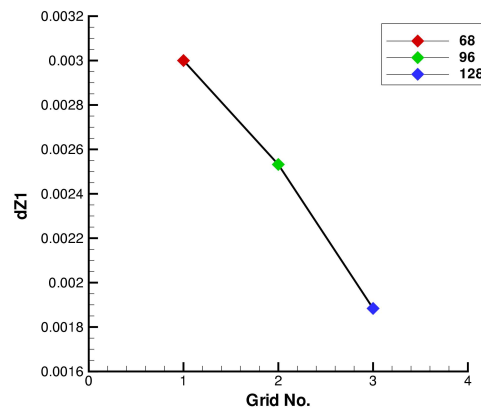


FIGURE 5.7: First wall normal point location in dimensionless height

In Figure 5.7 one of the most important parameters of the grid design is shown, that of the first point's distance from the wall. It's importance relies on the widely accepted fact in the CFD community that the distance of the first point from the wall plays a major importance to the correct capture of the boundary layer. However this will be investigated further when presenting the obtained results. A picture of each grid can also be found below for comparison and completeness.

Grid 1: Coarse Grid

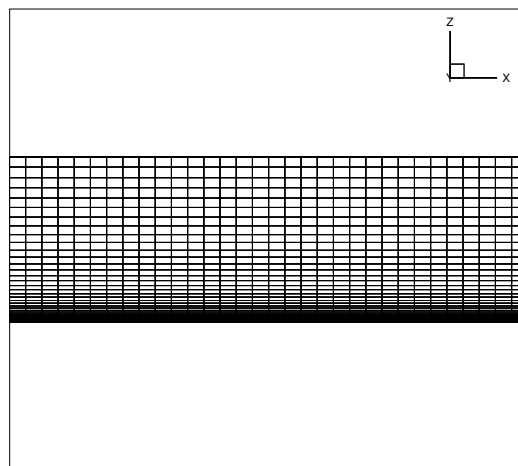
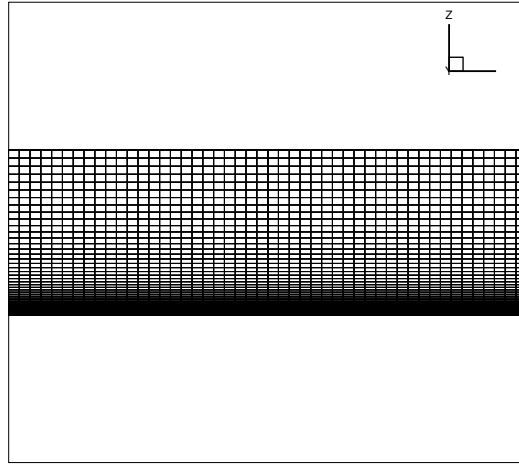
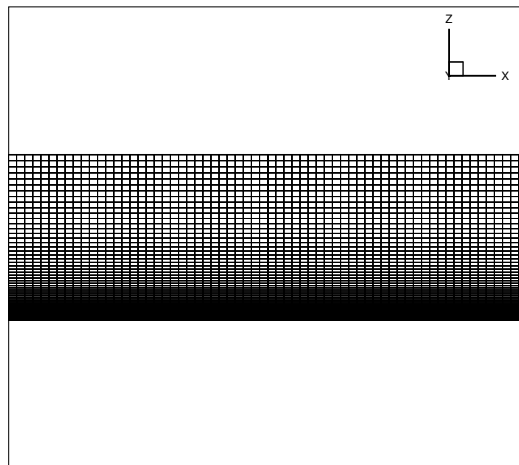


FIGURE 5.8: Coarse Grid $64 \times 48 \times 68$

Grid 2: Medium GridFIGURE 5.9: Medium Grid 96^3 **Grid 3: Fine Grid**FIGURE 5.10: Fine Grid 128^3

5.4 Results and Discussion

In this section, a selection of the most important results obtained from all the ILES simulations conducted using CNS3D will be presented and discussed. The order in which this happens will follow a logical path where on each step arguments are made in support for each decision taken. Eventually this will lead to the setup with the best results along with options for future work (see Chapter 7). Note that all computations presented

are simulated at a friction Reynolds number of $Re_\tau = 395$ using the same grid as in the LES simulation of [116] unless stated otherwise. All velocity component profiles plotted against DNS are nondimensionalised by the friction velocity obtained by the individual grid and limiter. Note that the DNS Re_τ plotted is the average value obtained during the fully developed stage of the simulation as a time accurate variation was not possible to obtain.

The statistical quantities are averaged over a long enough timeframe to ensure a statistical steady state. This is achieved by looking at the wall shear stress plots over time as seen in Appendix C, where all scales are adequately repeated. Also the simulation time after the flow is fully developed is such so that the mean velocity passes through the domain a sufficient number of times (usually at least 25 times) and therefore should ensure statistical convergence of the largest scales. First and foremost however, the reasoning behind the decision of using the forcing term to 'drive' the flow is given.

5.4.1 Massflux Conservation

The origin of the problem of maintaining the mass flux in the channel arises from a combination of issues. The most important being the combination of the periodic boundary condition along with the numerical and physical dissipation present in the numerics and flow physics respectively. If just periodic boundary conditions are used in the streamwise and spanwise direction, there is no 'driving' mechanism present to sustain the flow from stagnating due to thermal losses in the flow itself, especially if turbulent, and due to numerical dissipation. Therefore, a steady loss of the kinetic energy of the flow will occur and if run for enough time, will eventually lead to a stagnated flow.

Three simulations were run to prove this point, one without any mass flux preserving method, one with the periodic boundary mass flux preserving method and the third with a forcing term (see Section 5.3.3). The resulting mass flux variation in time is then plotted for each case on the same plot for easy comparison as shown in Figure 5.11. Note that for all cases in this section the Mach number used was $M = 0.5$ and using the MC limiter.

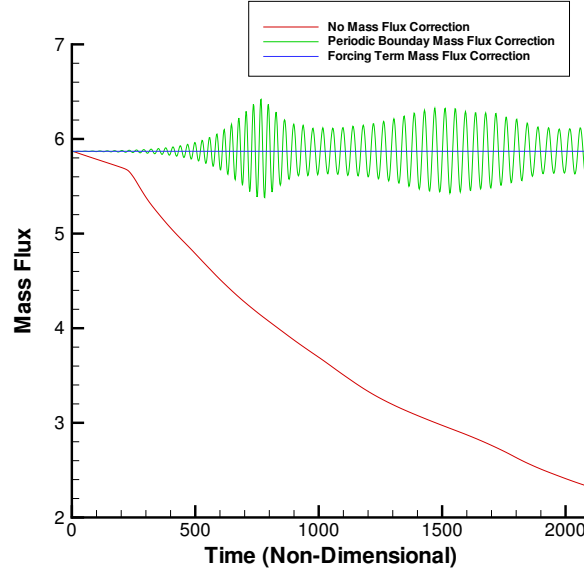
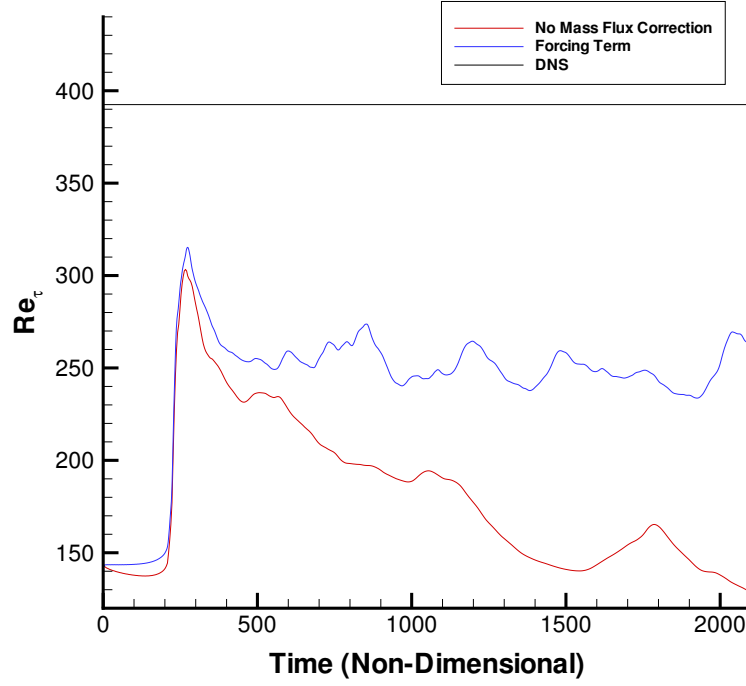


FIGURE 5.11: Massflux preservation methods investigated

It is evident from Figure 5.11 that a gradual decrease in the massflux occurs when no method to preserve it is used. On the other hand, the mass flux preserving periodic boundary condition presented in Section 5.3.3 and used in a considerable number of incompressible LES channel flow investigations ([20, 21, 42] to name a few), managed to maintain the massflux but unfortunately proved too unstable to use in the context of compressible flows. To further prove this point, there is no compressible channel flow investigation of any kind that has used this type of mass flux preservation. Next, the forcing term mass flux correction has been used in a number of compressible LES investigations ([52, 55, 112]), however at a higher Mach number of $M = 0.5$ usually. At this Mach number the flow is at a quasi-incompressible state and starts to exhibit some compressible flow features. However more on this topic is discussed in the next section.

FIGURE 5.12: Friction Re with and without forcing term

In Figure 5.12, the friction Reynolds number is plotted for with and without a forcing term. It is obvious from the simulation that although the flow developed to a turbulent state for both cases, the simulation without a forcing term eventually re-laminarised within the specific time window. From this it is concluded that a massflux preserving method is indeed required with the forcing term being the most suitable candidate. Note further that the most dissipative scheme employed was used in order to test the stability of the mass-flux conservation method and explains the poorly resolved friction Reynolds number.

5.4.2 Mach Number

The vast majority of channel flow simulation that have been conducted to date have used incompressible solvers. Most importantly all DNS simulations were computed using incompressible solvers, while only a small majority of the LES simulations used a compressible formulation of the NSE. In the compressible LES sources, the Mach number at which the simulations were conducted was $M = 0.5$. Although the flow is in a quasi-incompressible state, meaning that the density variations and temperature gradients start

to be of significance, the results obtained can still be compared in the nondimensional formulation provided that favre averaging is performed to the relevant flowfield variables.

However, it is noted that in all compressible ILES investigations conducted an adiabatic solid wall boundary condition was specified. This was obviously not required for the incompressible DNS simulations conducted since incompressibility does not allow for density changes or therefore temperature gradients. But the compressible LES investigations conducted at $M = 0.5$ specified the 'correct' value of temperature at the solid wall which can be interpreted as 'forcing' the correct solution. For this reason, all simulations are conducted using an adiabatic no slip wall condition so that the temperature obtained at the wall is given by purely the numerical method's abilities.

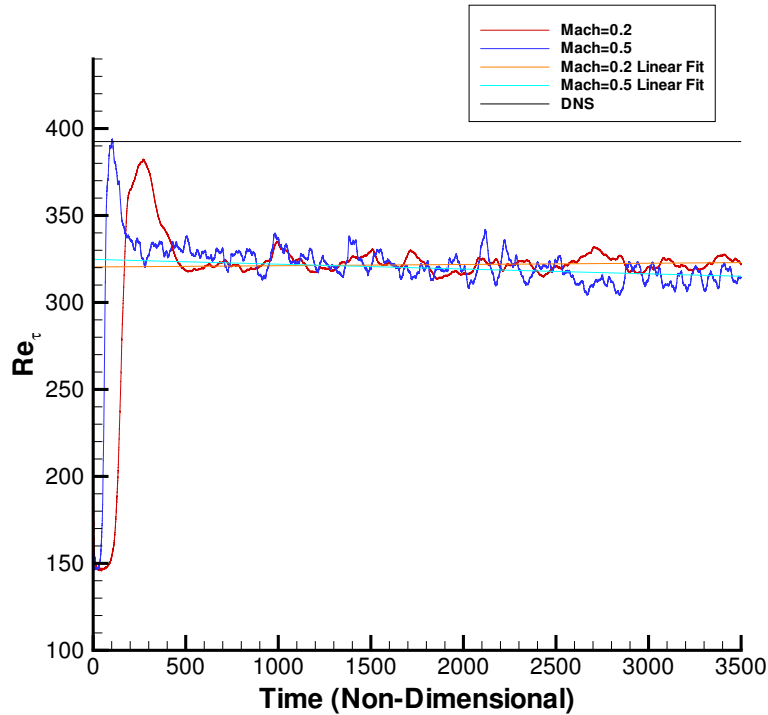


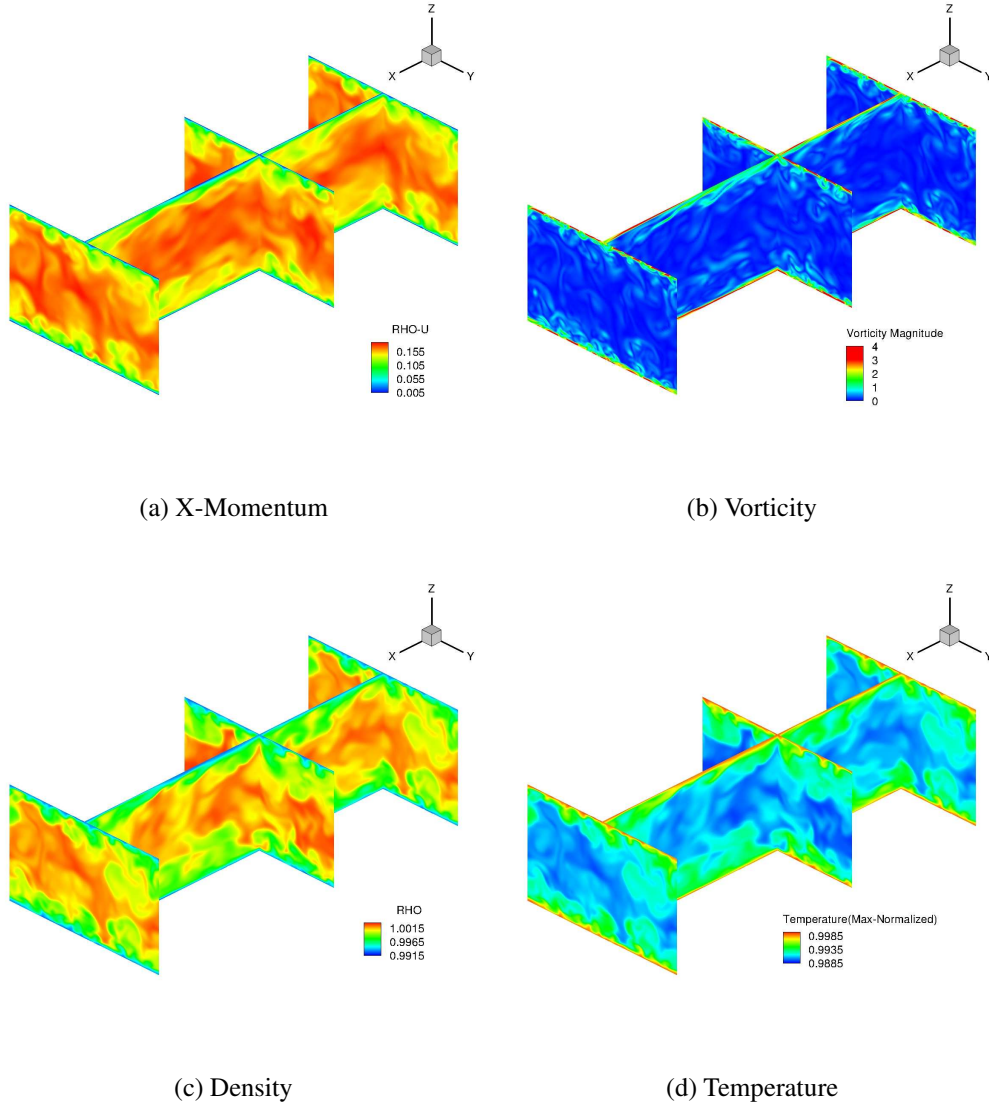
FIGURE 5.13: Friction Re obtained at different Mach number simulations

The graph in Figure 5.13 depicts the friction Reynolds number at two different Mach numbers, 0.2 and 0.5. In both cases, the WENO 9th order limiter was used and a line showing the mean value obtained for the developed part is depicted for each. A general trend can be noticed in the results for the Mach number equal to 0.5 case; there is a small but gradual decrease of the friction Reynolds number after the flow fully develops. This

was not the case for the near incompressible Mach number of 0.2 for which the flow maintained a steady mean value throughout the whole turbulent developed state. This result is somewhat surprising when taking into account that lower dissipation is expected at a higher Mach number. From this point forward, all results shown will be from simulations conducted at a Mach number of $M = 0.2$.

5.4.3 Flow Development & Characterisation

In this section some flow features of the domain will be presented. The total number of grids examined is three. The first one is of size (N_x, N_y, N_z) containing $64 \times 48 \times 68$ points respectively as equivalent to the one used in [116], and the second and third are custom for the case at 96^3 and 128^3 respectively. From this point forward, all results presented will be for the 128^3 size. The rest of the results for the other grids can be found in Appendix C.

FIGURE 5.14: Flow characterisation, 128^3 , WENO 9^{th}

From Figure 5.14(c) it is clear that the variation of density in the domain is within the incompressible density variation of a Mach number $M = 0.2$ flow and corresponds with the temperature variation Figure 5.14(d). The obtained maximum temperature variation is within the theoretical 4% from freestream, in particular the obtained max was well below at about 1.15% variation. It is observed that the highest temperatures are obtained at the solid wall regions as expected due to skin friction and thus leading to the lower densities noticed there too. In Figure 5.14(a)-5.14(b) the coherent turbulence structure can be seen and as expected are mainly located in the near wall region due to the no-slip wall.

5.4.4 Grid Dependency

In this section a grid dependency study is conducted using the WENO 9th order scheme since it gave the best results. The grids used for this study are the same three grids mentioned in Section 5.3.7. For the results of the remaining methods the reader is referred to Appendix C.

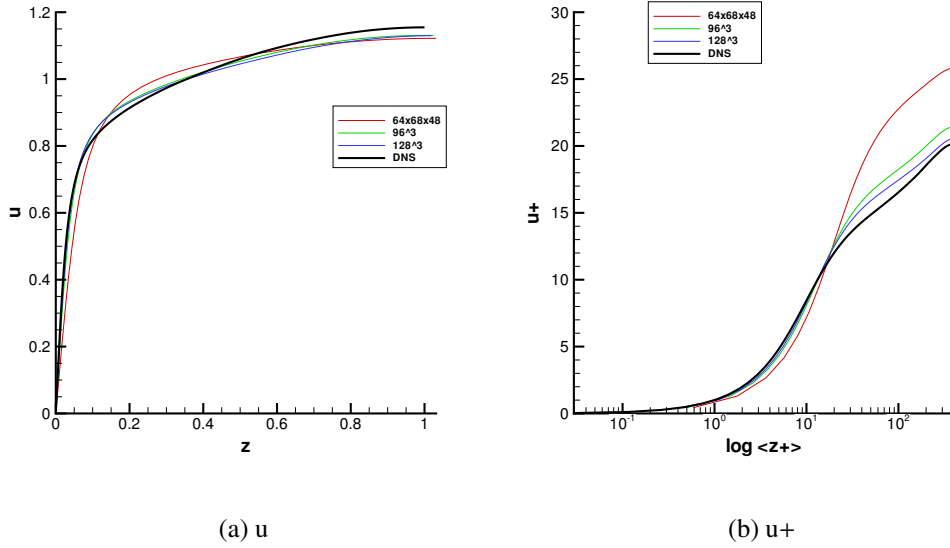


FIGURE 5.15: Streamwise velocity profile obtained on different grids using WN9 limiter

In Figure 5.15(a) the wall normal half-channel profile of the streamwise velocity normalised by the free-stream velocity is presented whereas in Figure 5.15(b) the streamwise velocity is normalised by the friction velocity u_τ . A small difference is noticeable in the mean streamwise velocity profile in Figure 5.15(a) between grids 2 and 3, however the thicker boundary layer for grid 3 is evident. In the case of ILES, the higher velocity just above the wall leads to a higher temperature and therefore lower density due to the compressible description of the NSE used. Hence, in order for the conservation of mass law to be met, a lower centreline velocity is required. This is the case for the resulting higher velocities obtained at the centreline as can be noticed in Figure 5.15(a). Further, the difference in the value of the velocity u divided by the friction velocity u_τ , that is u^+ , at the half-channel height between grids 2 and 3 shows that the 128³ grid was capable of obtaining primarily a better friction velocity u_τ and secondly a closer agreement to the

DNS velocity profile. The velocity profiles depicted are normalised by the friction velocity u_τ as already mentioned and since the streamwise velocity profile is of an identical value at the channel half-height in Figure 5.15(a), the difference at the same location in Figure 5.15(b) for u^+ can only be due to the difference in the value of friction velocity u_τ obtained.

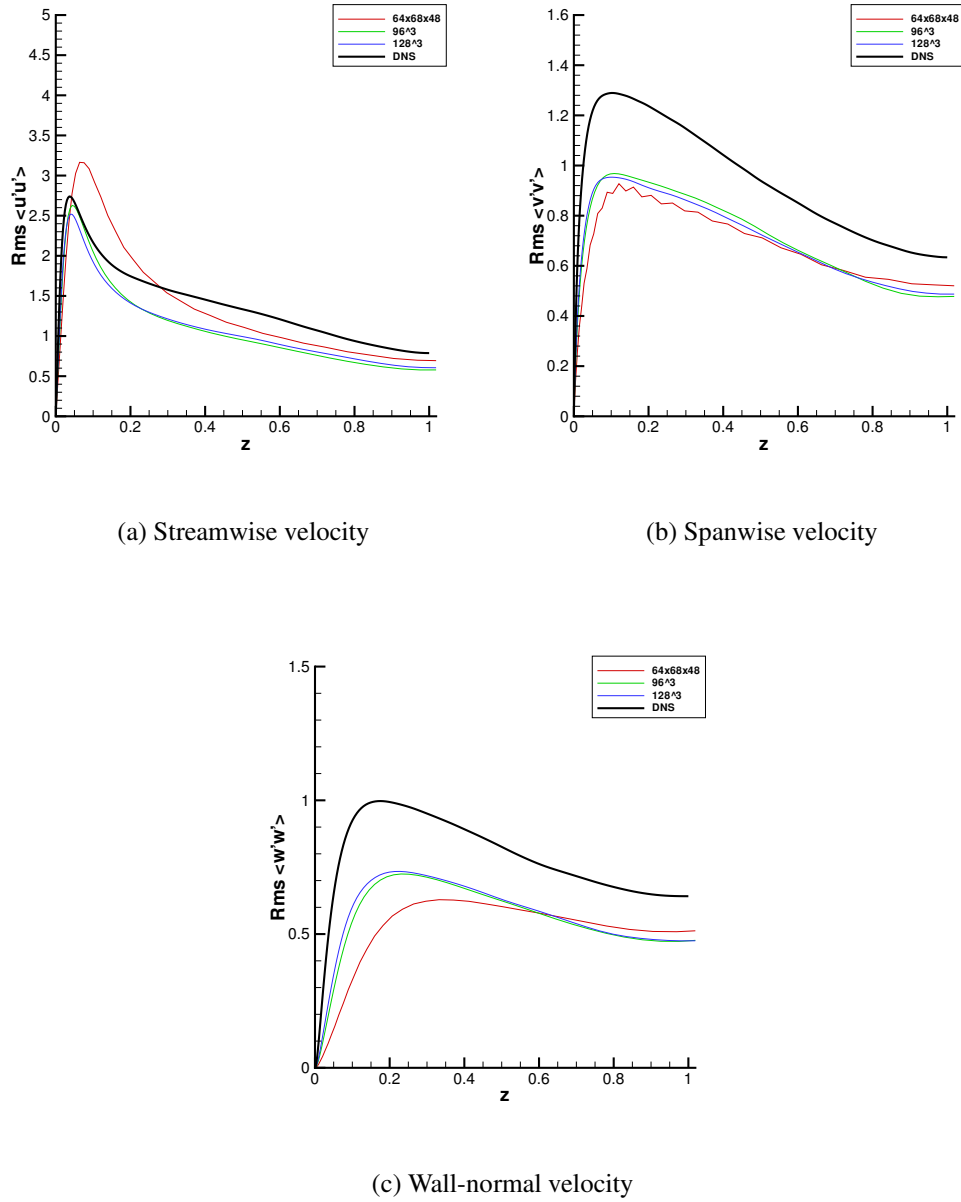


FIGURE 5.16: RMS of velocity components for WN9 limiter

The overshoot of the streamwise velocity Reynolds stress RMS in Figure 5.16(a) for grid 1 is due to the underprediction of the wall shear stress and not due to the overprediction of the actual value. However, the underprediction that occurs for grids 2 and 3 is a result of the streamwise velocity Reynolds stress RMS being of a lesser magnitude to that of DNS.

Also, the RMS of spanwise velocity as seen in Figure 5.16(b) using WENO 9th order on grid 1 is not smooth and instead an oscillatory behaviour is evident. The reason for this is the large stencil WENO 9th order requires (needs 5 cell-centre values to interpolate left and right states) when reconstructing the variables in combination with the fairly coarse grid being unable to resolve the spanwise direction adequately. Therefore there is a grid dependency for WENO 9th for which the solution develops an unphysical oscillatory behaviour on badly resolved flows and has also been confirmed by other investigations [97, 117].

For the spanwise velocity Reynolds stress RMS, the same trend is noticed as for the previous velocity components. That is, there is a significant improvement from grid 1 to 2 but relatively less from grid 2 to 3, with the main improvement being the better estimation of the maxima point position.

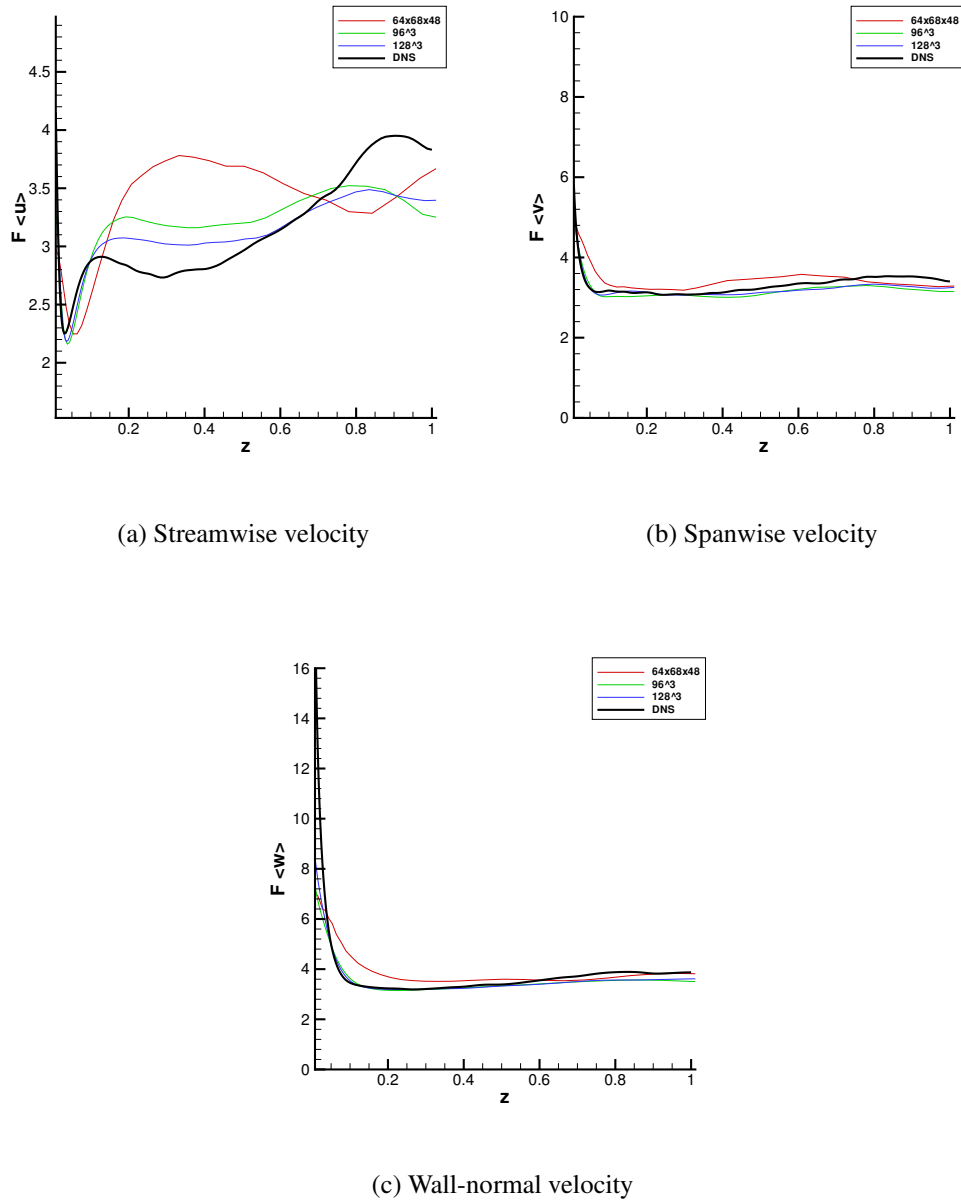
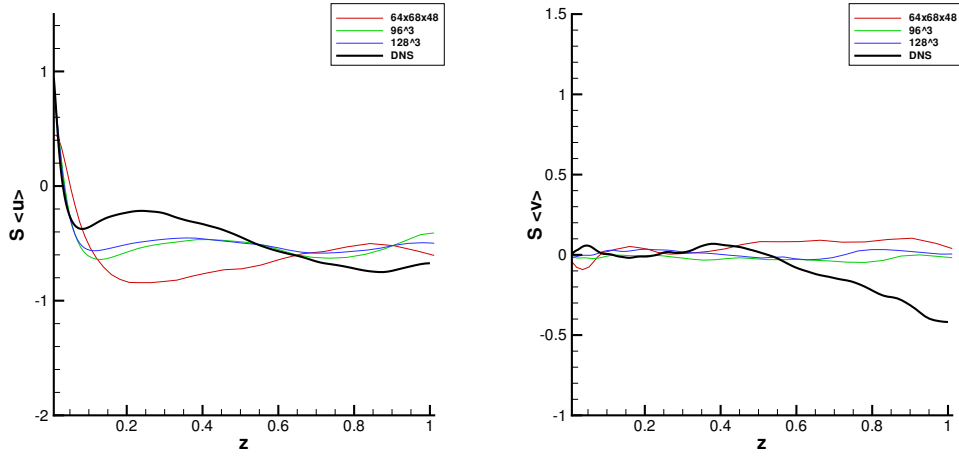


FIGURE 5.17: Flatness of velocity components for WN9 limiter

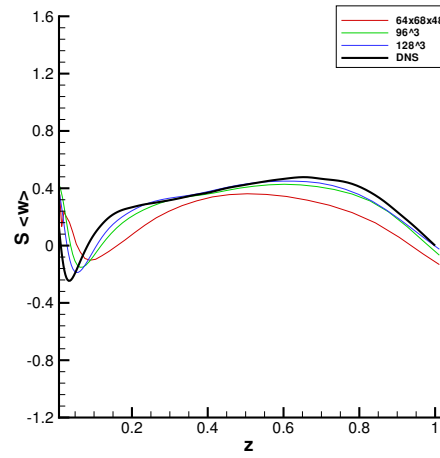
The sudden increase in the value of flatness for the wall normal velocity component indicates the highly intermittent character it exhibits near the wall. Grid 3 manages to obtain a value of around 8 whereas grids 2 and 3 are just below and over 6 respectively. This is where (higher order statistics) the finer grid, grid 3, proves to give considerably

better results than the rest, coarser grids. Though the streamwise velocity flatness is similar for grids 2 and 3, the rest of the profiles along the channel height show considerable improvement on grid 3 showing that the region is under-resolved still.



(a) Streamwise velocity

(b) Spanwise velocity



(c) Wall-normal velocity

FIGURE 5.18: Skewness of velocity components for WN9 limiter

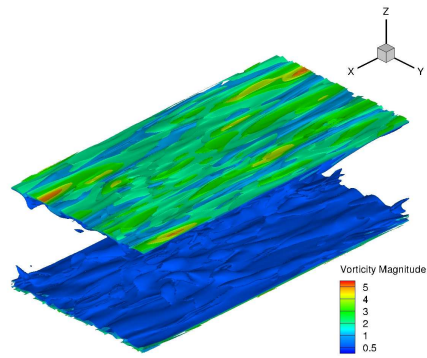
As can be seen in Figure 5.18, the skewness velocity component profiles for all grids

do not predict the near wall maxima point well. However the most important result obtained from the simulations and did not agree with those obtained from DNS for any limiter and grid is the spanwise velocity skewness profile as approaching the half-channel height. DNS predicts a sudden decrease in the spanwise velocity skewness which the current simulations have not managed to obtain. Note that the skewness is a sign sensitive statistic since the numerator is to the power of three. Thus it is possible that the ensemble and time average conducted is not enough for a reasonable amount of scales to exist for the particular statistic.

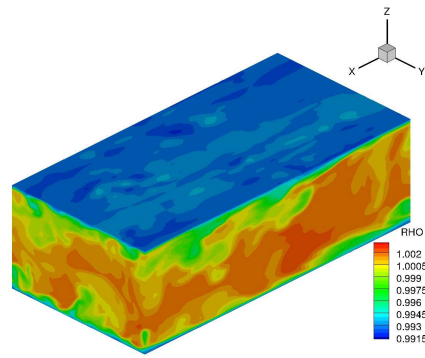
In all plots the improvement of the results from grid 1 to grid 2 is substantial whereas from grid 2 to 3 is much less. The main features and trends of the flow have all been captured adequately on the 96^3 grid already however the 128^3 still manages to improve the value of the friction Reynolds number Re_τ even further. This can be seen in Figure 5.15(b), where the value of u^+ in the mid-height of the channel is significantly improved due to the better estimation of the friction velocity u_τ . The general conclusion drawn here is that the 128^3 does give the best results out of all grids as expected, however the computational cost required is significantly larger than the 96^3 . The 96^3 required for example 12168 CPU-hours of computational time in order to complete a 2100 non-dimensional timeframe decomposed into 24 blocks whereas the 128^3 required 17280 CPU-hours of computational time for the same timeframe but having the domain decomposed into 32 blocks.

5.4.5 Numerical Scheme Effect

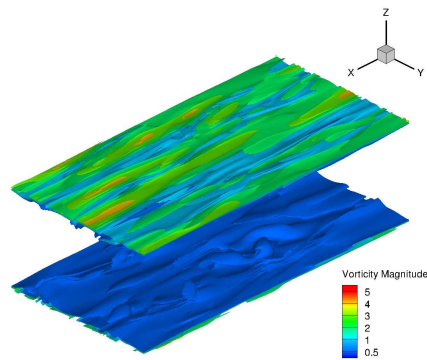
The effect of the numerical schemes is evaluated on 128^3 grid. The ability of each limiter on resolving three-dimensional turbulent structures is clearly visible in the iso-surfaces of vorticity and density contours depicted in Figure 5.19. It is evident that the solution obtained for WENO 9th order is considerably more turbulent since numerous and smaller scales can be observed in either density contour plots and vorticity iso-surfaces. The differences are harder to observe when comparing the MC limiter with the 5th order MUSCL limiter, however the maximum and minimum values of vorticity obtained were of a larger magnitude for 5th order MUSCL and even more for WENO 9th. The observations made from the flowfield vorticity iso-surfaces and density contours in Figure 5.19 are further justified by the following profiles given in Figure 5.20 - 5.23.



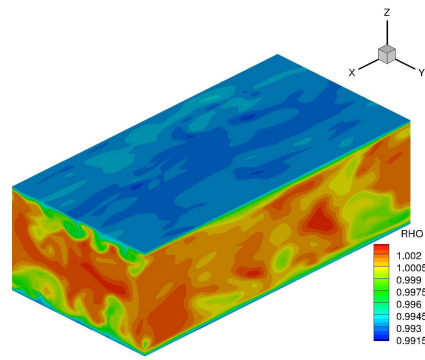
(a) Vorticity, MUSCL 5th



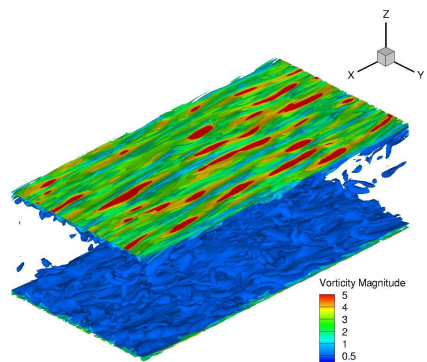
(b) Density, MUSCL 5th



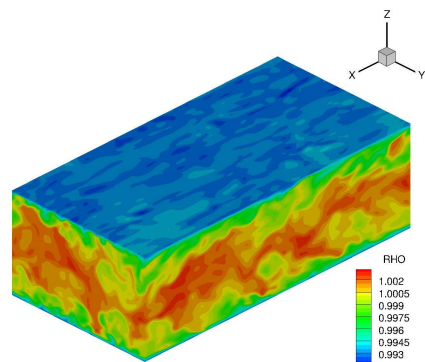
(c) Vorticity, MC



(d) Density, MC



(e) Vorticity, WENO 9th



(f) Density, WENO 9th

FIGURE 5.19: Flow characterisation, 128^3 grid

It is observed that the generation of vorticity occurs at the viscous region and is 'ejected' due to the low speed streaks into the boundary layer thus making it turbulent. This flowfield mechanism is responsible for producing hairpin vortices that get stretched by the ambient shear. These streamwise elongated hairpin vortices were also observed in the simulation conducted in [20, 118] where their shape was also found to be asymmetric.

The general trend noticed in all following plots is the ability of the WENO 9th order scheme to outperform all other reconstruction limiter methods utilised. This is in part due to the lower numerical dissipation introduced by the scheme itself thus allowing for a more turbulent flow.

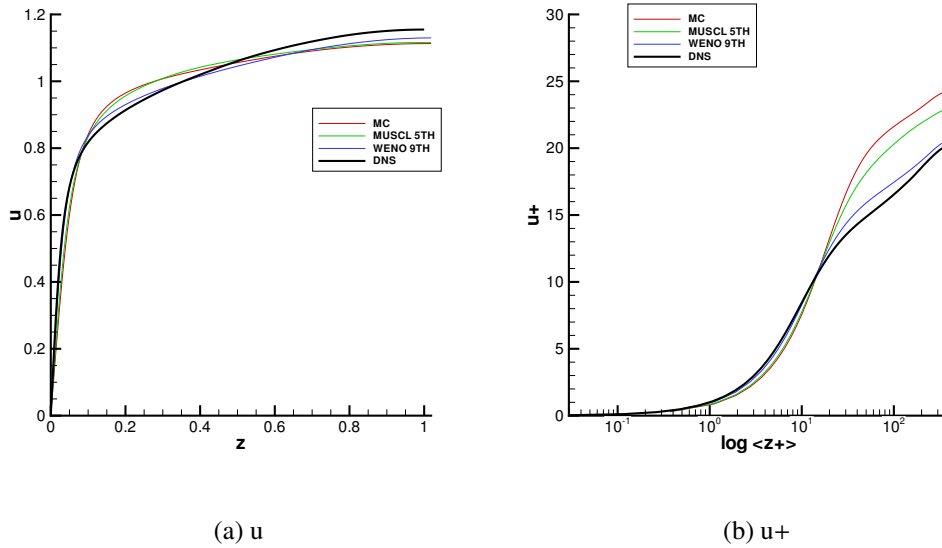


FIGURE 5.20: The effect of the numerical scheme on streamwise velocity profiles

In the velocity profiles in Figure 5.20(a) it can be seen that WENO 9th has given the best streamwise velocity profile, following that obtained by the DNS simulations very well. The MUSCL schemes also performed well with MC giving a better profile overall as seen in Figure 5.20(a) but the marginally worse u^+ in Figure 5.20(b) indicates that 5th order MUSCL managed to resolve the boundary layer better resulting in a higher friction velocity closer to that obtained in DNS. Next the profiles of the Root Mean Square (RMS) Reynolds stresses are plotted. The magnitude of these give a clear identification of the turbulent fluctuation strength. From all those plotted in Figure 5.21 it is evident that WENO 9th gives the best results out of all the limiters in this comparison as well. The

streamwise velocity Reynolds stress RMS is predicted very well again for WENO 9th actually capturing the distance from the wall where the maximum RMS occurs correctly. This was not the case in both MUSCL limiters, with the 5th order methods giving better results in terms of RMS peak and magnitude. For the spanwise and wall normal velocity, the RMS profiles obtained in all cases is lower than those obtained for DNS which is natural considering that these velocity components actually arise due to turbulent motion and can be regarded as a stronger turbulence criteria. In both cases, WENO 9th order returns the best values in terms of magnitude, distribution and peak point.

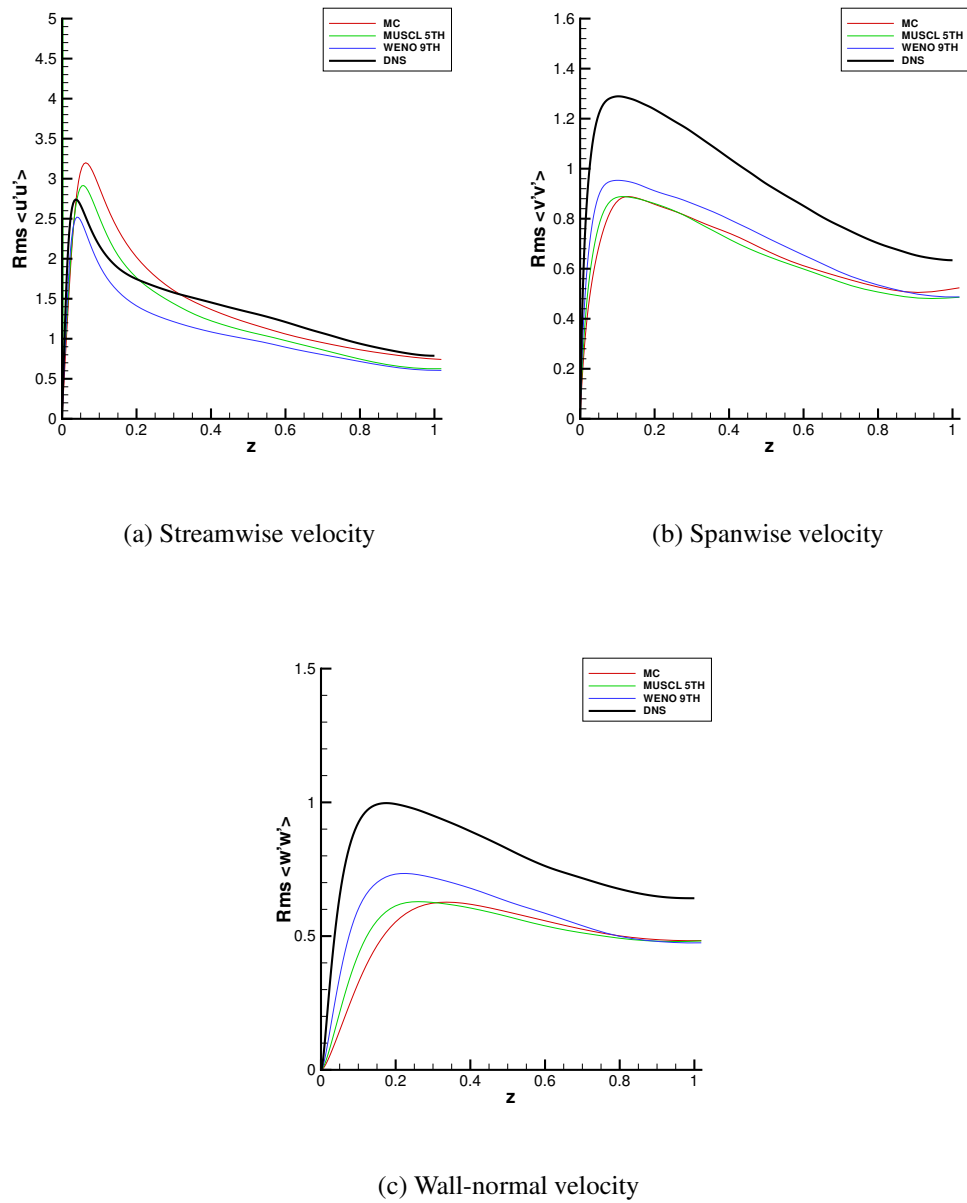


FIGURE 5.21: The effect of the numerical scheme on normalised RMS stresses (128^3 grid)

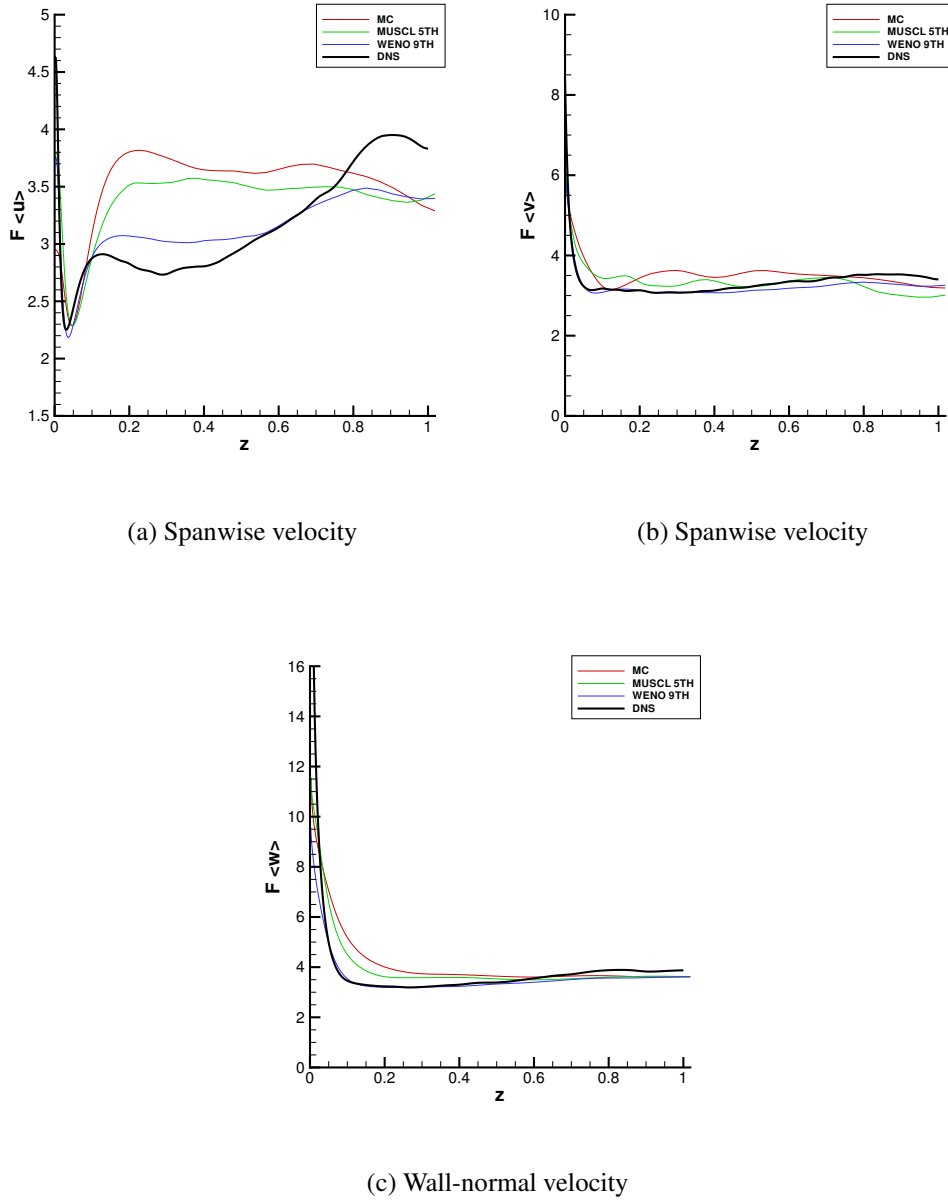
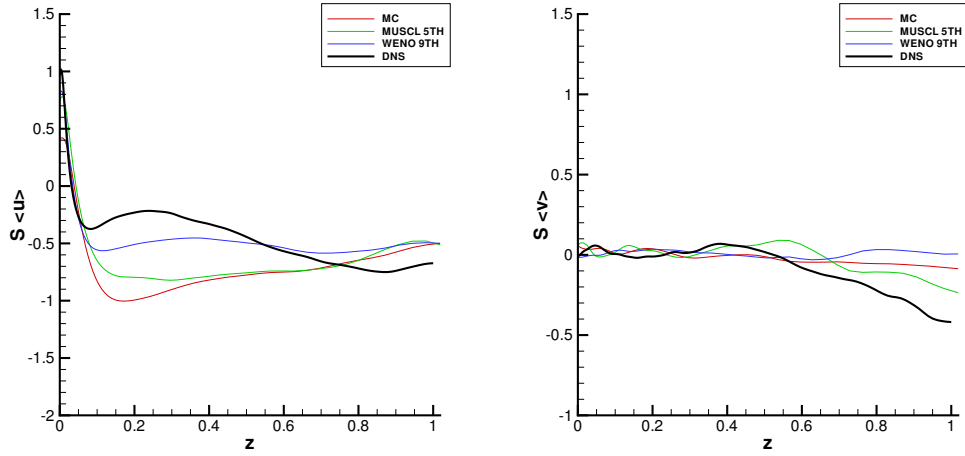


FIGURE 5.22: The effect of the numerical scheme on normalised flatness (128^3 grid)

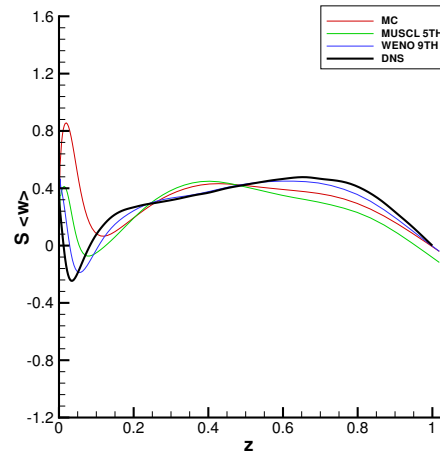
Higher order statistics are considered the hardest properties in the flow to obtain correctly. The reason for this is that they are obtained by higher order derivatives of the flowfield variables and thus are very sensitive to incorrect profiles and gradients of the flow. Here is where WENO 9th order excels over the other methods employed the most. It is the only reconstruction method employed that predicts the path of the streamwise flatness

profile correctly as well as the best in the spanwise component too, since the remaining methods have an unnatural long wave-like oscillation. In the wall normal velocity flatness profile, WENO 9th order is the only method to follow very closely the DNS solution.



(a) Streamwise velocity

(b) Spanwise velocity



(c) Wall-normal velocity

FIGURE 5.23: The effect of the numerical scheme on normalised skewness (128^3 grid)

In the case of the skewness velocity profiles it is clear that WENO 9th performs the

best in the streamwise direction, being able to capture the main shape of the DNS profile. On the other hand it fails to detect the drop in spanwise skewness around the half-height region of the flow like the MUSCL 5th order manages to do. However the best correspondence to the wall normal velocity skewness to those of DNS is given by the WENO 9th order method.

Furthermore the difference between the results obtained with the CBS and HLLC Riemann solvers has been investigated. In order to obtain the estimate of the maximum difference, the comparison has been performed on the coarsest grid where the effect should be more pronounced. The results summarised below for the MC limiter indicate that both Riemann solvers yield practically identical results with a negligible difference in the obtained velocity profiles (Figure 5.24). The slight advantage of CBS in the obtained RMS velocity components fluctuation as seen in Figure 5.25 cannot justify it being selected as the primary Riemann solver due to it requiring a longer time to compute. For this reason the HLLC approximate Riemann solver has been used in the simulations reported.

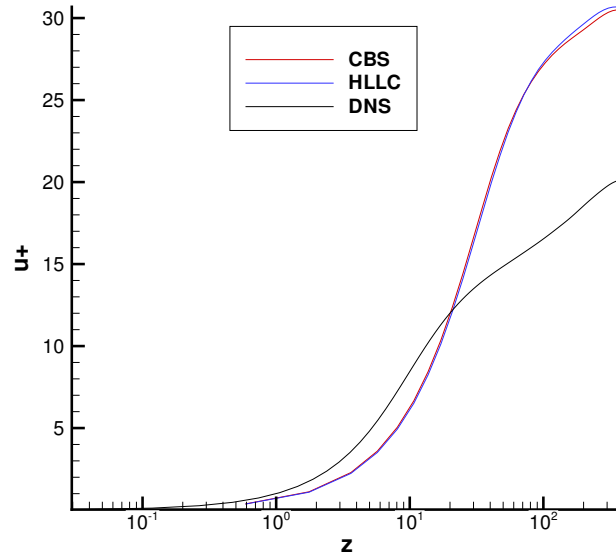


FIGURE 5.24: Comparison of HLLC and CBS Riemann solvers, u^+ vs $\log(z)$

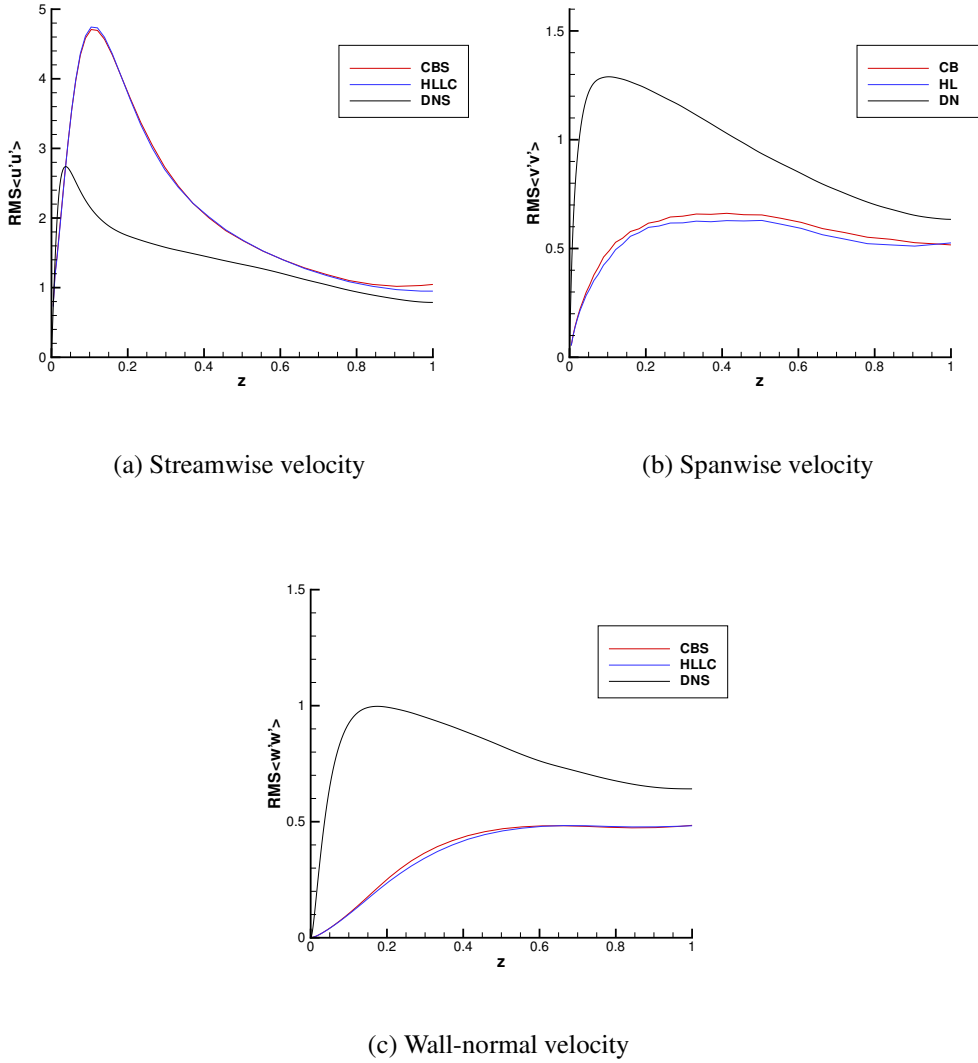


FIGURE 5.25: RMS of velocity components for CBS and HLLC Riemann solvers

5.4.6 Low Mach Number Treatment Effect

The Mach number of $M = 0.2$ is considered to be relatively low for a compressible solver and as discussed in Section 4.4 a novel approach is used in order to minimise the excessive numerical dissipation that occurs. It is worth noting that the majority of the flow and more importantly the boundary layer is of an even lower local Mach number, with the $M = 0.2$ region obviously only appearing far from the wall around the centreline of the channel. The results presented in this section will be based on those obtained for the 128^3 grid

using the WENO 9th order limiter along with the novel method presented in Section 4.4.

From the contour surfaces plotted in Figure 5.26, the major impact the LMNT has on the resolution of turbulent scales is clear. Finer turbulent vorticity structures can be noticed in all the flow region, even at the half-height channel region which previously barely had any vorticity iso-surfaces at all. The density contours act as an indication that the solution is still physically 'sane' since the variation in value in the domain is still within the incompressible range. The improvement of the results however becomes further obvious when comparing the various statistical profiles done next.

Possibly the most important advantage of using LMNT is it's ability to produce results on a coarse grid equivalent to those on a finer one not using LMNT. The streamwise velocity profile (see Figure 5.27) of both MUSCL type limiters on grid 1, give results equivalent of the same reconstruction method on grid 2 without LMNT. This is not observed in the case of WENO 9th order although the result on grid 1 is greatly improved.

However a weird phenomena occurs in grids 2 and 3 for which the application of LMNT resulted in an overprediction of the friction velocity. This can be noticed by the lower u^+ velocity in the half-height of the channel due to the lack of enough dissipation. In this case the lack of dissipation can be attributed to the scheme not being dissipative enough as well as the fact that grids 2 and 3 are finer and therefore result in even less dissipation. These, coupled with the fact that LMNT can actually be regarded as a 'blending' of a second order central scheme that is dispersive by nature, starts to suggest that the scheme in general begins to exhibit dispersive numerical phenomena.

This is validated further by observing the RMS profiles (Figure 5.28) for WENO 9th on grids 2 and 3 when using LMNT. Although the near wall RMS profile of the wall normal velocity is in excellent agreement with DNS, soon after it starts to deviate, remaining at a constant higher value. Fully turbulent DNS channel flows conducted at higher Reynolds numbers [35], did not produce profiles of the same unusual trend proving that the turbulence overprediction is introduced due to unphysical numerical modelling. Similar trends are noticed in the flatness and skewness profiles, however with the difference that the latter returns towards the DNS profile at the end of the half height.

Since the simulations were the overprediction of turbulence did not return any unphysical results it can be deducted that the numerical method is under-dissipative in the high frequency turbulent scales captured due to the finer grid. This could be thought of as a flow containing higher total energy than normal in the small scales and thus possibly effecting the energy transfer from the larger scales. Concerning both MUSCL limiters,

the LMNT implementation causes the profiles to obtain DNS-like characteristics even on the coarse grid 1, with the finer meshes improving the profiles in the near wall region mainly.

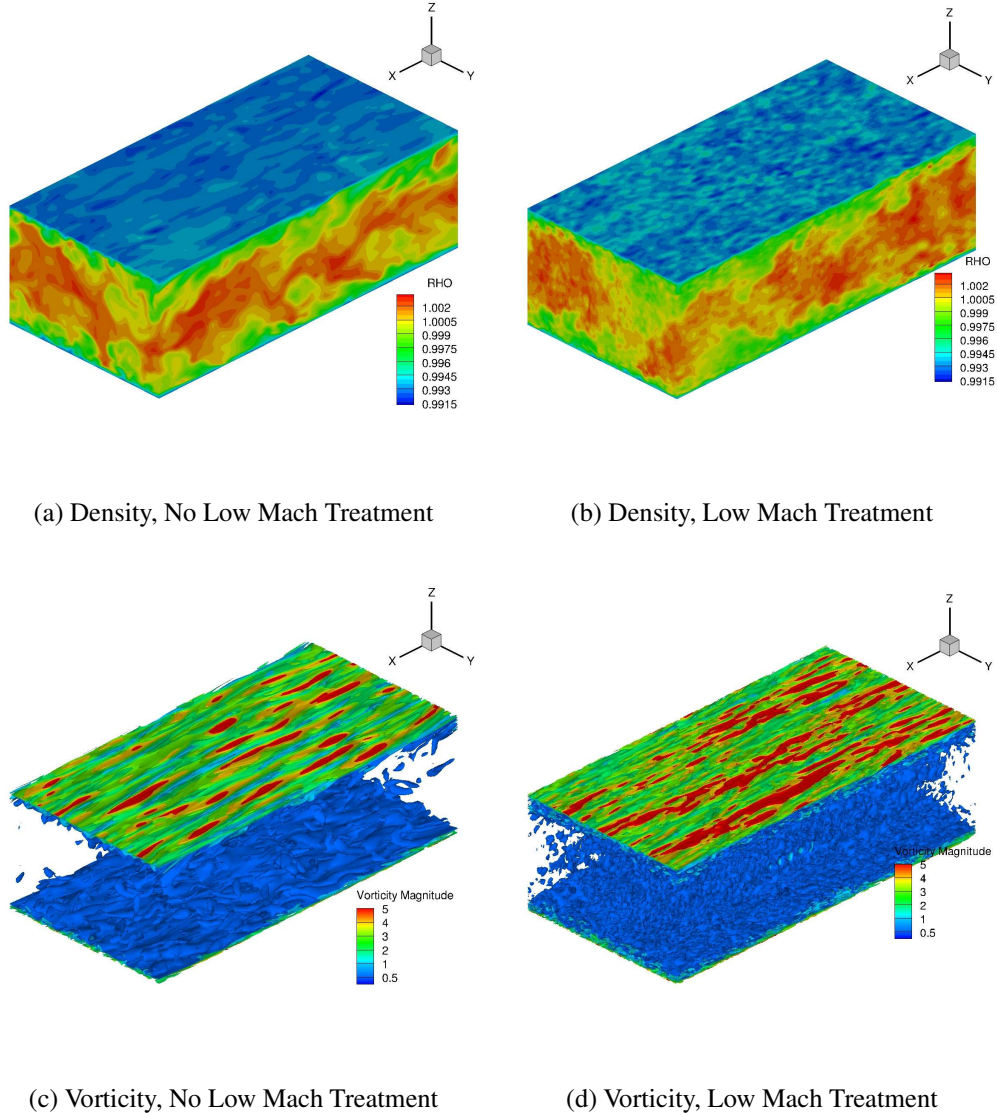


FIGURE 5.26: Effect of Low Mach Number treatment on small-scales resolution, 128^3 grid, WN9 limiter

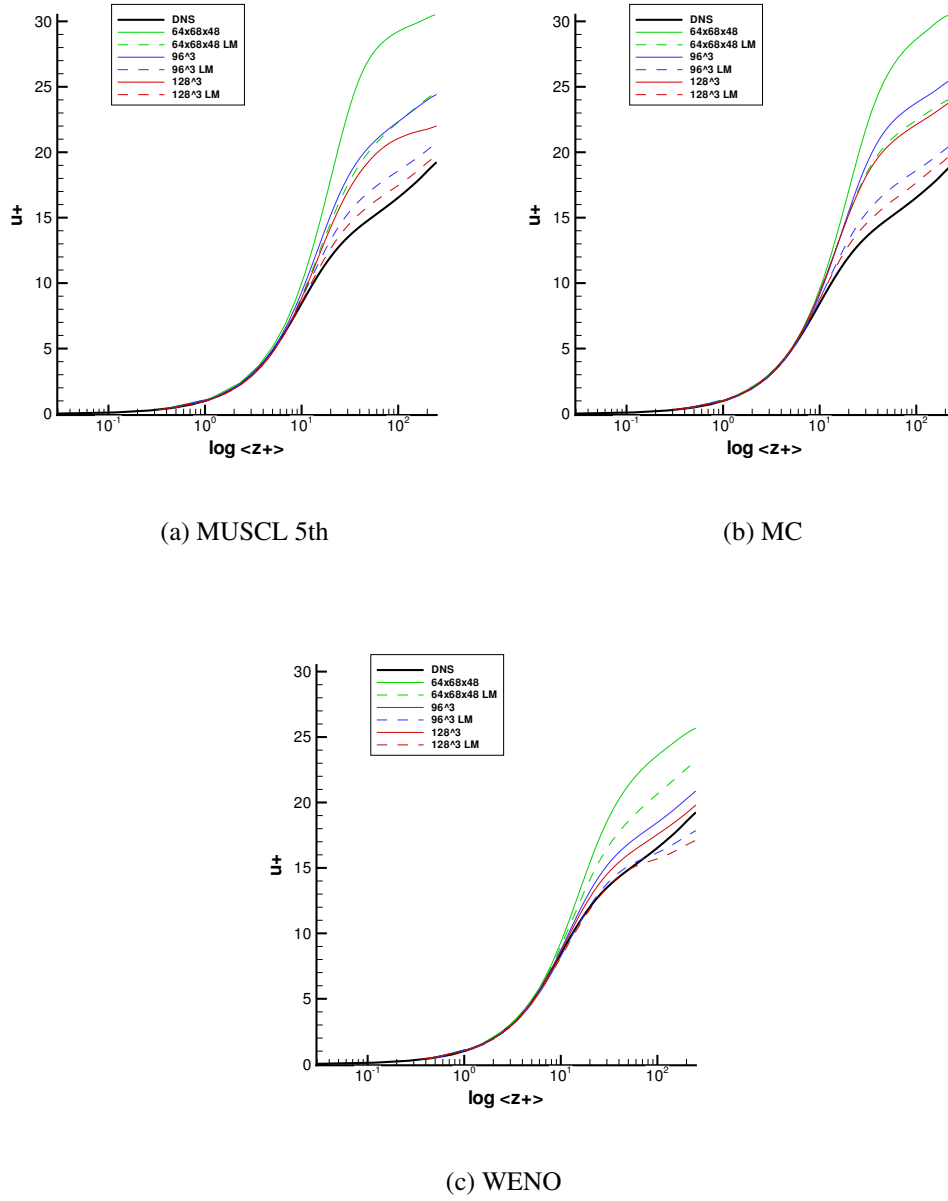
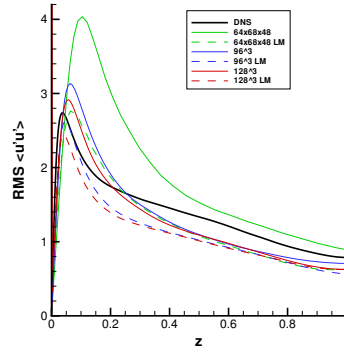
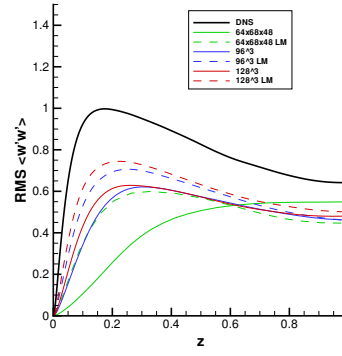


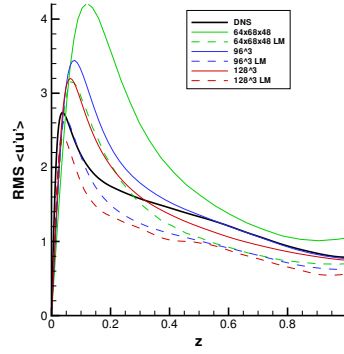
FIGURE 5.27: The effect of LMNT on the normalised velocities



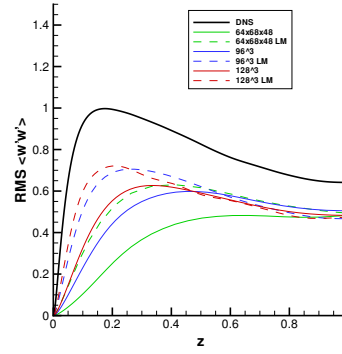
(a) MUSCL 5th



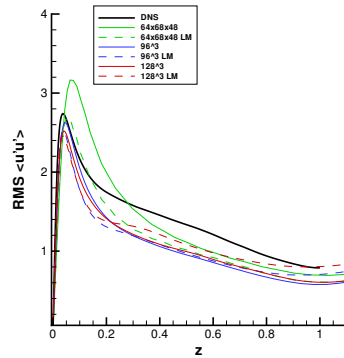
(b) MUSCL 5th



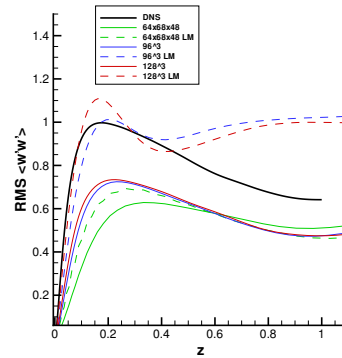
(c) MC



(d) MC

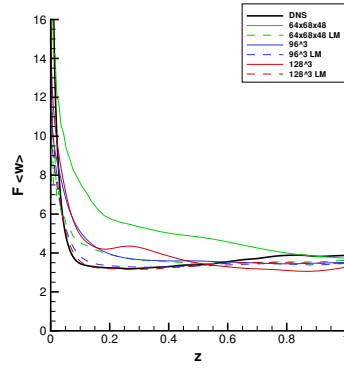


(e) WENO 9th

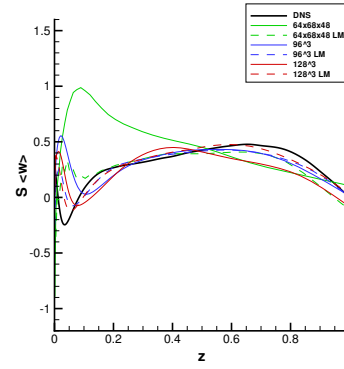


(f) WENO 9th

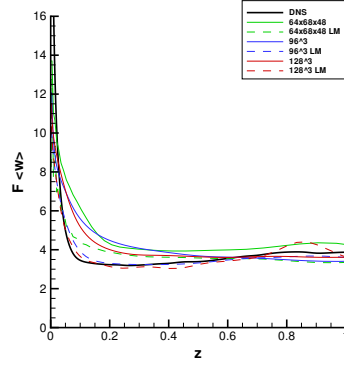
FIGURE 5.28: The effect of LMNT on the normalised RMS stresses



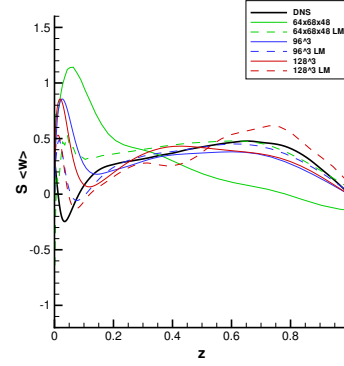
(a) MUSCL 5th, flatness



(b) MUSCL 5th, skewness



(c) MC, flatness



(d) MC, skewness

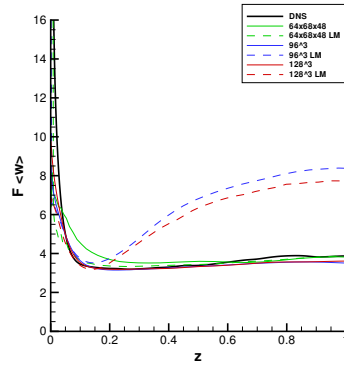
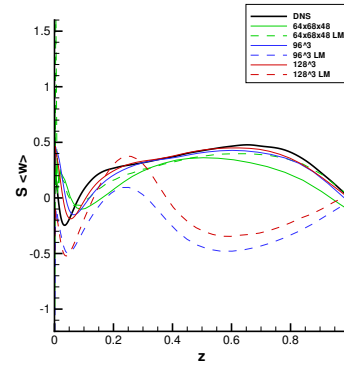
(e) WENO 9th, flatness(f) WENO 9th, skewness

FIGURE 5.29: The effect of low-Mach number treatment (LM) on the flatness & skewness of the wall-normal velocity

5.4.7 Summary of Wall Friction

Since the near wall region of the channel is of main importance, one of the most suitable flow parameters to compare in this context is the friction Reynolds number Re_τ which is a good indicator of the velocity field obtained right above the wall. In particular, the friction Reynolds number depends heavily on the obtained (resolved) boundary layer which in turn effects the temperature field and thus viscosity. Therefore a lower value of friction Reynolds number is an indication of a poorly resolved boundary layer which in this case translates to a lower intensity turbulent flow than required. All the values obtained for Re_τ with or without LMNT and using different limiters and grids can be seen in Table 5.2 below. The time history graphs of the friction Reynolds number that were used in order to obtain the values below can be found in Appendix C. From Table 5.2, the improvement of the obtained Re_τ when using LMNT is evident. MUSCL 5th and MC struggle to keep up with the 9th order WENO that manages to obtain fairly decent results. Note that the VL limiter was also tested from the available second order reconstruction limiters, however MC from the same category of limiters outperformed it and therefore was dropped out from the subsequent calculations. Also the friction Reynolds value obtained in the incompressible DNS simulation of $Re_\tau = 395$ was actually slightly less at $Re_\tau^{DNS} = 392.25$

Grid: 68 (Hickel)				
	Re_τ	$\sigma(Re_\tau)$	LM: Re_τ	LM: $\sigma(Re_\tau)$
MUSCL 5th	247.6034	8.5190	304.4846	4.8818
Monotonized Central	249.6553	18.2322	304.8508	7.2902
WENO 9th	293.7590	5.8061	342.1258	3.9405
VL	230.4412	4.9067	N/A	N/A
Grid: 96				
MUSCL 5th	306.8990	6.6710	353.5113	4.4251
Monotonized Central	291.8033	4.1950	353.1977	4.0139
WENO 9th	352.8386	2.9911	398.2815	6.6746
Grid: 128				
MUSCL 5th	328.4557	7.4667	372.5895	3.3804
Monotonized Central	307.8864	6.1183	367.0869	3.6829
WENO 9th	370.5519	3.8907	415.7984	4.7710

TABLE 5.2: Summary of time-space averaged Re_τ results

It is noted that WENO 9th order without LMNT provides as good results as MUSCL

5th and MC limiters with LMNT. So naturally the question arises of which of the aforementioned combinations is the most efficient. The WENO 9th order method required 183 hours to cover a nondimensional time length of 1400 units on 24 decomposed blocks using parallel computing (MPI protocol). For the same configuration MUSCL 5th and MC both with LMNT required just over 148 hours of computing time each, thus making the LMNT-MUSCL scheme combination favourable. Further, the implementation of the LMNT with WENO 9th order starts to overpredict the value of the friction Reynolds number Re_τ . In [119] the exact same reconstruction methods were investigated for a homogeneous decaying turbulence in a triply periodic cube and it was found that the WENO 9th order was the least dissipative of all methods. This leads to the conclusion that the numerical dissipation of the scheme in conjunction with the fact that finer grid resolutions resolve more turbulent scales eventually leads to an insufficient amount of numerical dissipation required to dump out the oscillations introduced by the LMNT because of its second order central discretisation method. Further, approximately the same friction Reynolds number is obtained between WENO 9th order without LMNT and MUSCL 5th or MC with LMNT on the 128^3 grid. For this case the domain was decomposed into 32 blocks and run for a total of 2100 non-dimensional time units. WENO 9th required a total of 540 hours of computational time whereas MUSCL 5th and MC either with LMNT required an estimated 410 hours, a considerably less amount of time.

Thus the 'blending' of the LMNT and MUSCL schemes seem to have performed well and actually converged towards the DNS value of Re_τ with increasing grid refinement. The maximum variation of the friction Reynolds number ($\sigma(Re_\tau)$) during the fully developed turbulent state is also shown in Table 5.2. This is an indication of the ability of the method in sustaining a constant turbulent intensity once developed. In this respect it is worth mentioning that the MC limiter on the coarse grid without LMNT had the largest value, meaning that the friction velocity at the wall fluctuated considerably during its fully developed turbulent state. From this respect, MC was not as stable in maintaining its developed turbulent intensity as MUSCL 5th although MC managed to get a slightly higher mean friction Reynolds number overall. The addition of LMNT managed to help 'stabilise' the turbulent intensity of the MC limiter in the coarse grid, another advantage of using LMNT apart from improving the general turbulent properties of the solution.

However, there is a downside to LMNT as well. It appears that when the scheme and grid do not introduce adequate dissipation, the numerical dispersion of LMNT overwhelms the solution and eventually leads to a numerically stable solution, which exhibits

unphysical behaviour in both friction velocity and higher order statistics. In preliminary runs [120] using WENO 9th order it was found that the application of LMNT in a triply periodic decaying turbulence in a cube resulted in less dissipation being introduced at the high wave number speeds when compared to the Kolmogorov cascade. This observed behaviour, which is more pronounced on fine grids correlates well with the findings presented in this chapter.

6

Compression Ramp

6.1 Introduction

So far in Chapter 5, all flows considered have been in the incompressible flow regime ($M = 0.2$). A few test cases run, showed that at quasi-incompressible flows of $M = 0.5$, compressibility effects start to appear and the need for an isothermal no slip condition is maybe required to stabilise the flow near the wall. Since most practical applications requiring numerical modelling in aerodynamics and in a lot of engineering applications require a compressible flow description, a test case is selected to examine this flow regime as well.

At high Mach number, the flow often exhibits strong unsteady flow phenomena such as unsteady flow separation, shock-turbulence and shock-boundary layer interaction which cannot be properly predicted by RANS solutions. In [57] and [58] the status of RANS simulations was summarised for compression corner flows. It was observed that no RANS model was capable of accurately predicting many aspects of the flowfield. Specifically, the RANS solutions did not display the unsteadiness of the separation shock, which was regarded as a major flaw and the source of the disagreement with the experimental mean

surface pressure. On the other hand, the use of DNS in high Mach number flows at the current point in time is in practise to industry infeasible, firstly due to the high Reynolds numbers one may come across and/or secondly due to the more relatively prohibiting complex geometries.

A more computationally cost effective method is LES, that as already mentioned, models the smaller scales of turbulence and thus is possible to apply on much coarser meshes than DNS while at the same time producing time accurate solutions unlike RANS. The strong unsteady flow phenomena experienced in high Mach number compressible flows require a time accurate solution to be able to model correctly. This is in direct contrast to RANS that uses the time average effects of most scales to model them and seems unable to deal with the particular regions of interest. Furthermore, most effort put into developing SGS models for LES was and still is in the majority of cases conducted for incompressible solvers, leaving the compressible list of SGS to just a few. Thus the applicability of ILES to model turbulence in supersonic compressible flows will be examined.

In [59] ILES was also employed to compressible isotropic turbulence and it was concluded that the influence of the numerical dissipation is considerable and most shock-capturing schemes examined were unable to mimic the SGS dissipation correctly. However, it was also recommended that any SGS turbulence model is to be avoided on the grounds that the numerical dissipation of the schemes is relatively larger than the dissipation added by a SGS and is therefore 'masked' in any case. The investigation in [59] did not cover viscous fluxes or either inhomogeneous turbulence. A wide list of cases for simulating such compressible flows can be found in [60] where the literature survey conducted was exhaustive resulting in a plethora of cases and configurations.

From the available options, a compression ramp is proposed as an investigative case. This is a standard CFD validation case for turbulent boundary layer-shock wave interaction. The flow consists of a supersonic turbulent boundary layer of thickness δ in equilibrium approaching a compression corner defined by an angle α_{cc} . The deflection of the flow by the corner generates a shock system which for a sufficiently large pressure rise, causes the boundary layer to separate and a λ -shock to form. An example can be seen in Figure 6.1 below.

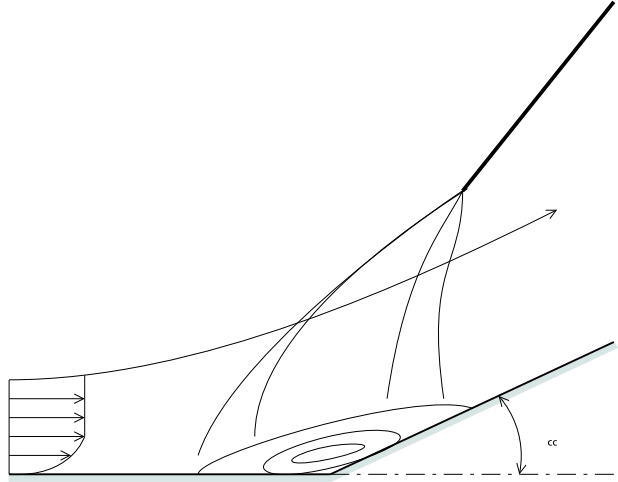


FIGURE 6.1: Compression Ramp

6.2 Compression Ramp Investigated Configurations

For the compression ramp configuration selected, the following flowfield and grid parameters are known [60]:

6.2.1 $Mach\ 3$, $\alpha_{cc} = 18^\circ$

Since a numerical investigation was being conducted, it was vital to compare against other numerical methods and approaches to determine any differences in the resulting flowfield. Since the case presented above included both various LES studied and DNS results it was selected to meet this purpose. It was not possible to find in the literature a compression ramp set-up that included LES, DNS as well as experimental results.

TABLE 6.1: Available data for $Mach\ 3$, $\alpha_{cc} = 18^\circ$

Reference	Data	M_∞	$Re_\delta \times 10^4$
[121, 122, 123]	DNS	3	2.1
[124]	DNS,LES	3	2.1
[125]	LES	3	2.1

TABLE 6.2: Computational details for $Mach\ 3$, $\alpha_{cc} = 18^\circ$

Reference	Type	Grid	SA	TA
[121, 122, 123]	DNS	$1000 \times 180 \times 80$	5th	3rd
[124]	DNS	$451 \times 151 \times 81$	6th	2nd
	LES-S	$451 \times 151 \times 81$	6th	2nd
	LES-D	$451 \times 151 \times 81$	6th	2nd
[125]	LES	$334 \times 91 \times 31$	6th	3rd

6.3 Methodology

6.3.1 Problem Description

The domain size of the case to be simulated can be seen in Figure 6.2.

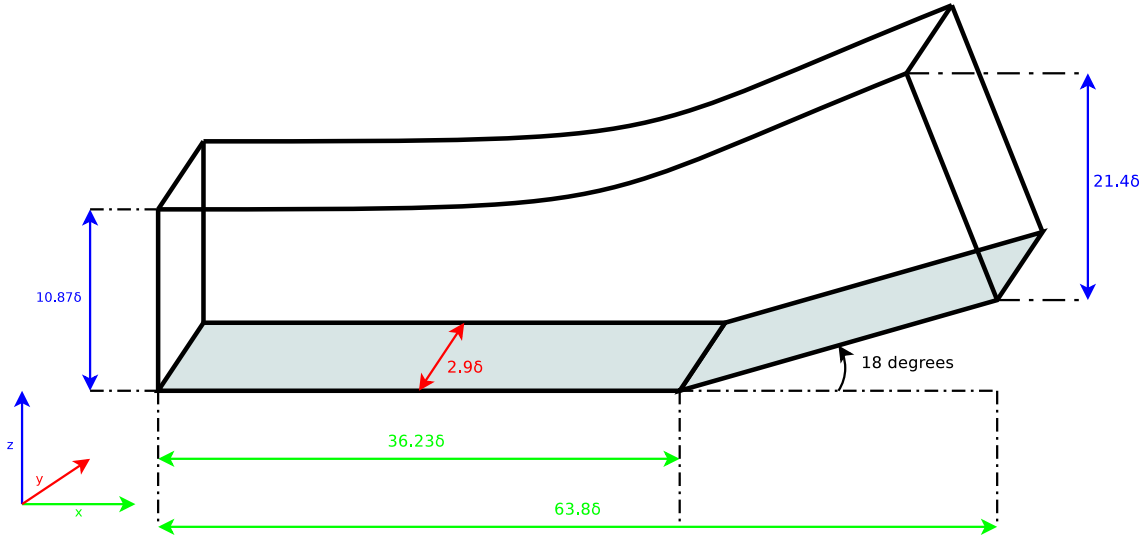


FIGURE 6.2: Compression ramp dimensions

The main problem with setting up a compression ramp simulation is the boundary condition for the inlet. If the inlet flowfield is incorrect, there is no hope of obtaining correct results. In all cases that have been simulated, a turbulent boundary layer has been used. However, the way the turbulent flowfield inlet is obtained is of concern. In the DNS simulation conducted in [121, 122], the turbulent boundary layer was obtained from an equivalent DNS of a flow over a flat plate. The location of the turbulent boundary layer

thickness equal to one non-dimensional height was located and an adequate time length of samples was taken to accommodate for all turbulent scales. The data was then used as inflow conditions for the compression ramp test case in a recursive manner.

The next two simulations in literature for the same set up are both LES [125, 126]. The manner in which the turbulent inflow condition was obtained in either case is similar as to the DNS test case but with the additional obvious step of having to filter the DNS data to the LES grid. It should be noted that the LES simulation of [126] used a half channel configuration as a pre-developing stage for the flow before it entered the flat plate. However, in the context of an LES simulation, it is best to try and avoid having to conduct lengthy DNS simulations in the first place along with outputting any data for use as inflow conditions taking up a considerable amount of storage.

A novel method is employed here, which is slightly different but similar to the above methods and avoids many of their 'shortcomings' as well as being at the same time more 'numerically' correct. The idea is based on the half channel pre-developing stage as used in [126] but in this case the flow enters directly into the compression ramp, skipping completely the flat plate DNS simulation. However the correct set up for the half channel domain has to be careful, and the conditions used in [126] were reconsidered for a number of reasons as will be discussed about later. A schematic depicting the general coupling method can be seen in Figure 6.3.

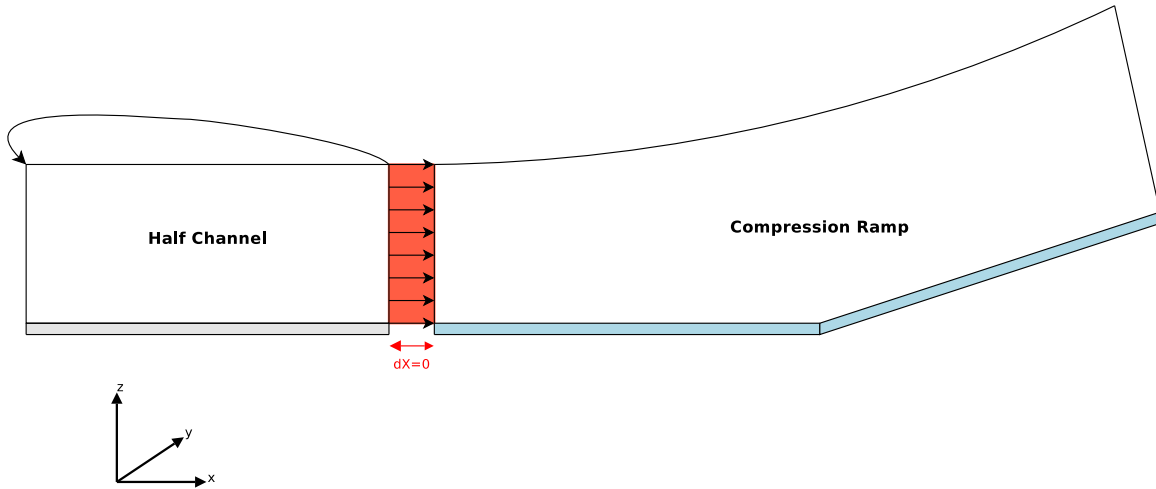


FIGURE 6.3: Half-channel compression ramp coupling

The general idea is simple. The half channel section is used in a similar manner as in the channel flow investigation conducted in Chapter 5 and is used to obtain a turbulent

flow. The difference is that only one side is solid wall and is the reason it is referred to as a half channel domain in this case. The set up is similar to that in Chapter 5, with the additional difference that the outflow is passed to the inlet of the compression ramp too.

From Figure 6.3, it follows that a half channel domain is used in order to obtain a turbulent profile which is then also passed as an inflow boundary condition to the compression ramp. This can be considered as numerically 'smoother' since the turbulent profile entering the compression ramp is of the same LES simulation and thus turbulence capability.

The first problem to be faced is the size of the domain of the half channel. Here, the dimensions of the ramp section were used in order to derive the dimension for the half channel region. The height and spanwise dimensions are taken equal to those of the ramp but the question is the streamwise length. For this, the following assumption is taken; that the length from the inlet of the compression ramp to the corner of the ramp used in the DNS simulations of [121, 122] should be sufficient to contain all turbulent streamwise scales. The corresponding domain size can be seen below in Figure 6.4.

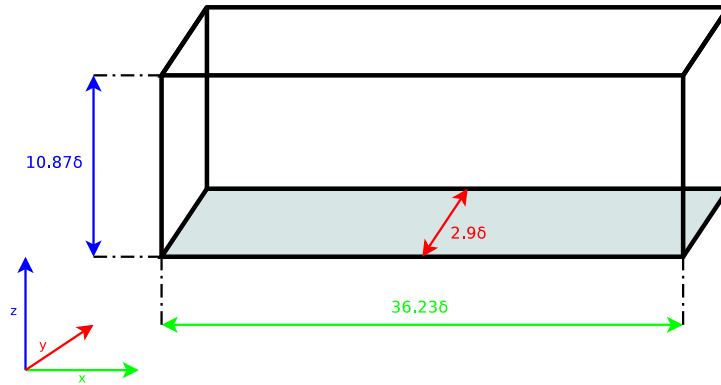


FIGURE 6.4: Half channel dimensions

6.3.2 Boundary Conditions

In the spanwise direction, typical periodic boundary conditions are used whereas in the streamwise direction, the inflow boundary condition is modified as the outlet of the half channel section and the compression ramp outlet as a typical supersonic outlet boundary condition as formulated in Equation (6.2). In the wall normal direction, an isothermal no-slip boundary condition is used for the lower section as in the DNS simulation [121, 122] whereas on the upper boundary a variety of BC's are investigated for reasons to be stated.

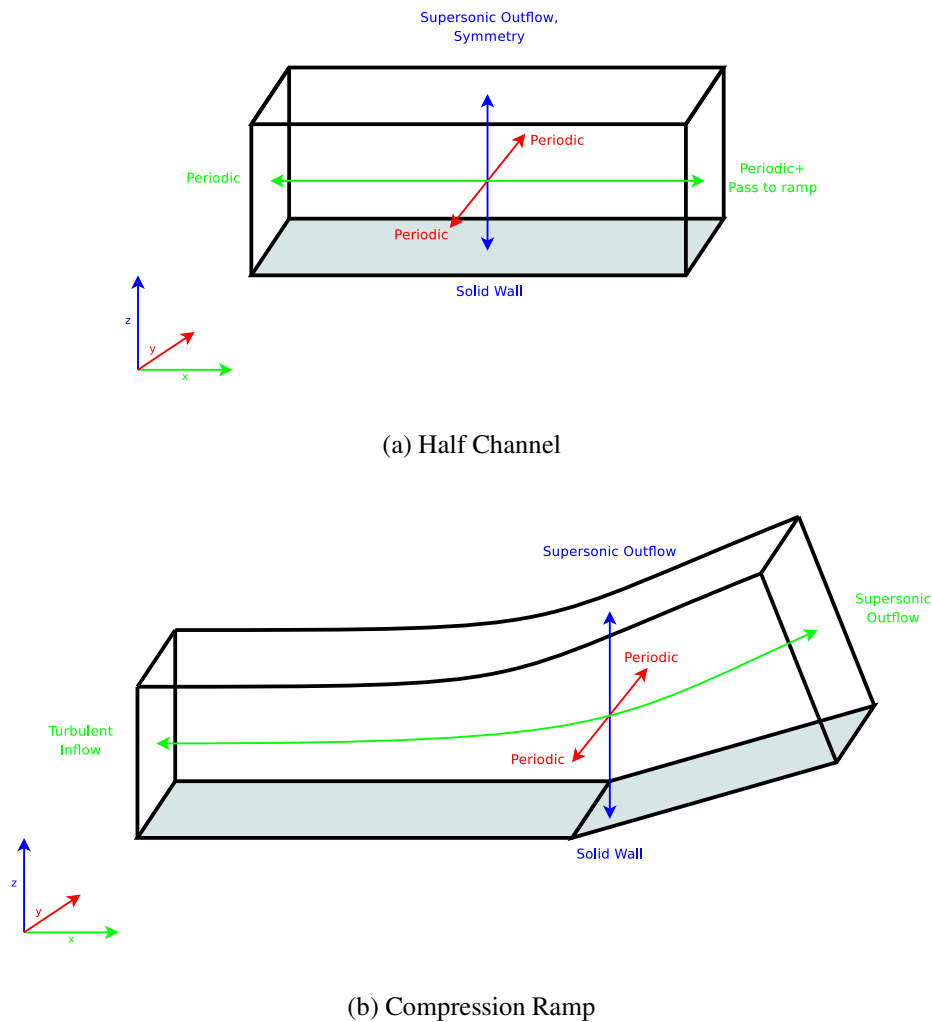


FIGURE 6.5: Full half channel and compression ramp boundary conditions

The boundary conditions applied can vary, based on numerical or physical considerations. The ideal case is where both numerical and physical approaches to choosing the boundary conditions converge, but unfortunately this may not always be the case. The set up employed here is one of these cases. From a physical point of view, it is expected that the flow should be at its farfield (freestream) properties before it has reached the top end of the domain, that is the end of the domain opposite the wall. However due to the numerical modelling, this may not always happen. In [126], the boundary condition located at the upper part of the half channel domain, was chosen to be symmetry, which is depicted in Figure 6.6(a) and formulated in Equation (6.1) below. A general overview of the applied boundary conditions for the half channel and compression ramp section can

be seen in Figure 6.5.

Note that since the z -axis is in the wall normal direction, the k -index will be used to illustrate the boundary conditions in Equation (6.1)-6.2.

- **Symmetry** In this case all the variables are mirrored in the x - y plane while the normal to the surface velocity is additionally changed direction in order to give a zero flux to the x - y plane, giving the symmetry effect. Note that the indexes reflect cell centres and are based on the notation given in Figure 3.6 in Section 3.3

$$\begin{aligned}
 \rho_k &= \rho_{KE2-(k-KE1)} \\
 \rho u_k &= \rho u_{KE2-(k-KE1)} \\
 \rho v_k &= \rho v_{KE2-(k-KE1)} \\
 \rho w_k &= -\rho w_{KE2-(k-KE1)} \\
 \rho E_k &= \rho E_{KE2-(k-KE1)}
 \end{aligned} \tag{6.1}$$

- **Supersonic Outflow** Here all the flowfield variables are linearly extrapolated outwards depending on the linear gradient of the flow just before the outlet. This translates mathematically to

$$\vec{W}_k = 2 \times \vec{W}_{k-1} - \vec{W}_{k-2} \tag{6.2}$$

A graphical schematic of the effect of each boundary condition can be seen below.

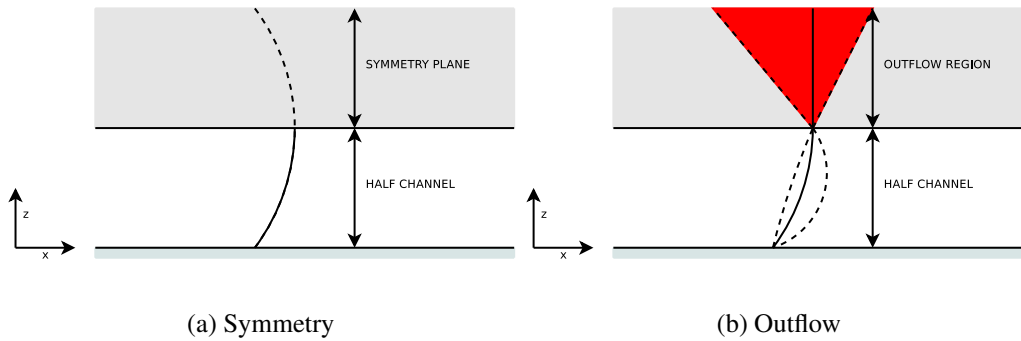


FIGURE 6.6: Half channel upper boundary conditions

It is widely known in the CFD community that the choice of boundary conditions can seriously effect the numerical results obtained and thus the choice can have great

impact. However since it is hard to predict the ability and the corresponding results of a simulation, for completeness all conditions were tested.

At this point it is important to mention that the choice of boundary conditions in the half channel, will effect the choice of the boundary condition in the compression ramp section too since only in the simulations conducted in this survey, are the half channel and compression ramp directly coupled. It is not possible for example to have a symmetry boundary condition in the half channel and use a farfield condition in the compression ramp section, due to the numerical discontinuity introduced at the boundary interface between the half channel and compression ramp.

Further, it is not clear to what degree a forcing term is required when the boundary condition at the top is farfield, since the (constant) freestream velocity prescribed could be sufficient to maintain the massflux. It is shown however, that the numerical dissipation is stronger when dealing with periodic boundary conditions in the streamwise direction and therefore a mass flux preserving method is still required.

6.3.3 Initial Conditions

The initial conditions used for the compression ramp and half channel section are similar with a couple of differences. First, the half channel domain includes a perturbation parameter which was shown in Chapter 5 to help develop a turbulent state considerably faster. Secondly, the compression ramp section velocity components take into account the local grid streamwise gradient in order to produce a smooth flow along the solid surface while the spanwise velocity is taken to zero. In either case, the streamwise velocity profile is considered turbulent and a statistically steady turbulent profile equation is used to generate it's [6] boundary layer profile:

$$u_{turb} = u_{\infty} \left(\frac{z}{\delta} \right)^{1/7}$$

where $u_{\infty} = U_m$ is the freestream velocity, δ is the boundary layer height and z is the distance of the cell centre to the solid wall. Note that this equation is used for up to a value of z equal to 1 since that is the height of turbulent boundary layer thickness used in the DNS simulations [121, 122] for the inflow. The initial condition for the half channel

is given by:

$$\begin{aligned}
 \rho(t=0) &= 1 \\
 u(t=0, z) &= u_m \left(\frac{z}{\delta}\right)^{1/7} \quad \text{if } z \leq \delta \\
 u(t=0, z) &= u_m \quad \text{if } z > \delta \\
 v(t=0, z) &= s\varepsilon \times u(t=0, z) \\
 w(t=0, z) &= s\varepsilon \times u(t=0, z) \\
 E(t=0, z) &= \frac{p}{\gamma-1} + \frac{\rho}{2} (u^2 + v^2 + w^2)
 \end{aligned}$$

where ε is a perturbation constrained by $\varepsilon \in [-1, 1]$, u_m is the freestream velocity, p is the pressure and s is the percent of perturbation. The resulting profiles for $s = 10\%$ can be seen below in Figure 6.7

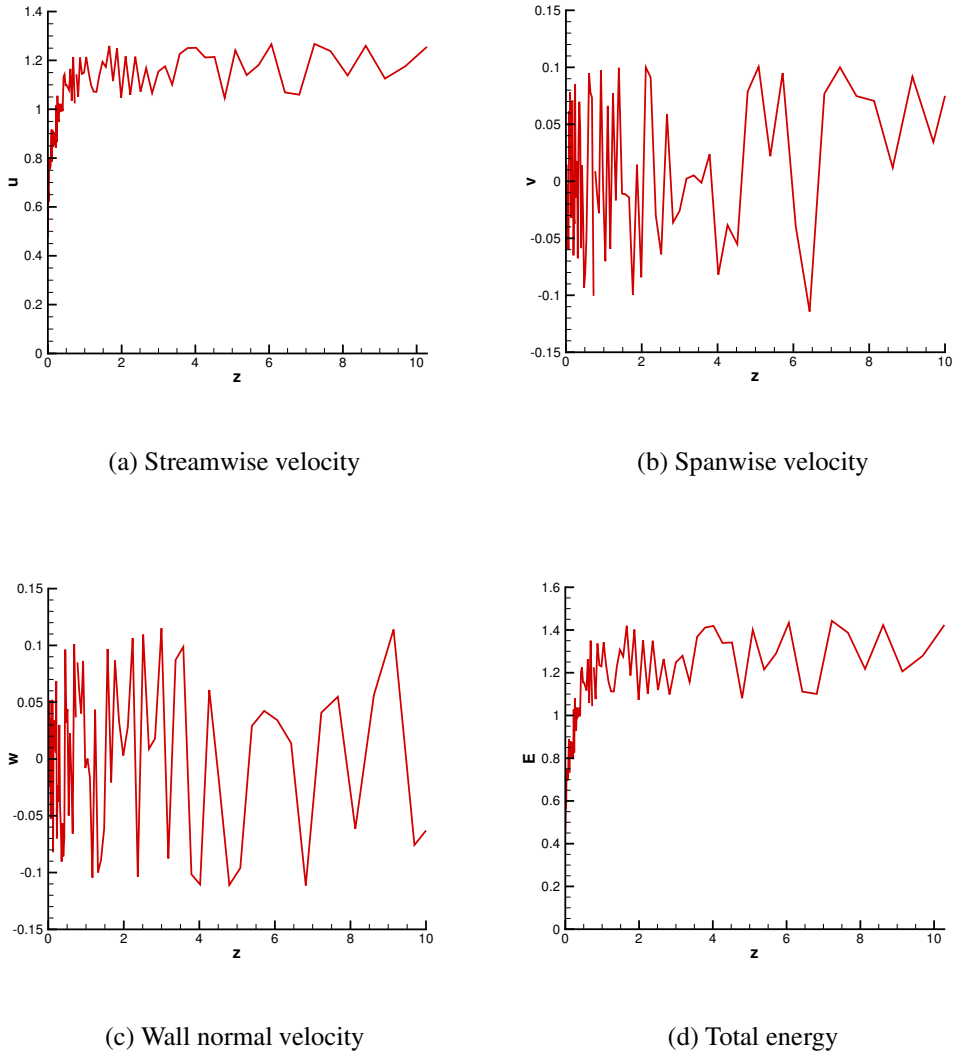
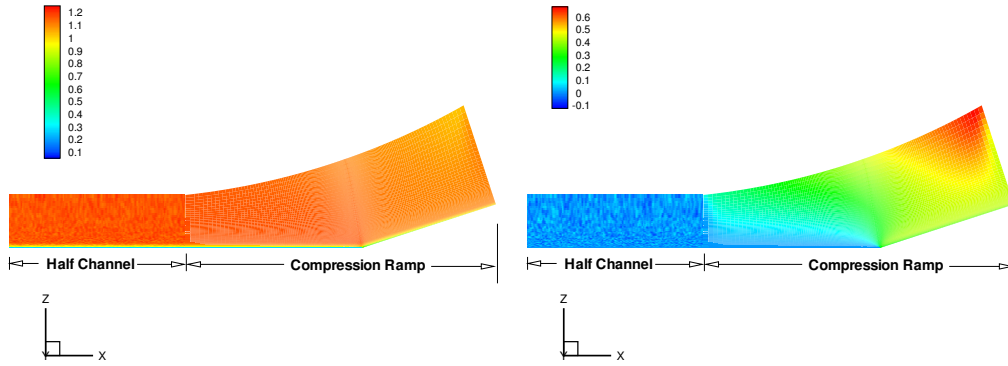


FIGURE 6.7: Half channel initial profiles

The initial condition for the compression ramp is given by:

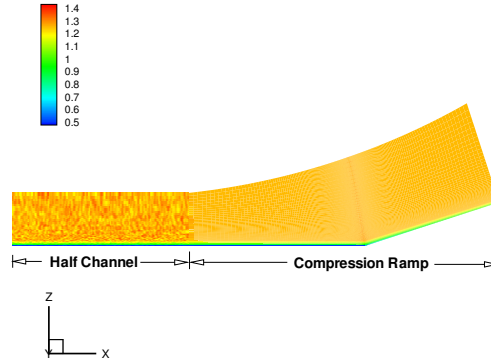
$$\begin{aligned}
 \rho(t=0) &= 1 \\
 u(t=0, z) &= U_m \left(\frac{z}{\delta}\right)^{1/7} \times \sin \Phi \quad \text{if } z \leq \delta \\
 u(t=0, z) &= U_m \times \sin \Phi \quad \text{if } z > \delta \\
 v(t=0, z) &= 0 \\
 w(t=0, z) &= u(t=0, z) \times \cos \Phi \\
 E(t=0, z) &= \frac{P}{\gamma-1} + \frac{\rho}{2} (u^2 + v^2 + w^2)
 \end{aligned} \tag{6.3}$$

where $\Phi = \text{atan}(r)$ and $r = \frac{\Delta z_{i+1/2}}{\Delta x_{i+1/2}}$. Since the density and spanwise velocity do not change, there is no point in plotting any graphs of their initial condition. Further, due to the local initial condition depending on the streamwise grid slope, a contour plot of the initial condition of the streamwise, wall normal velocity and total energy are given instead of vertical plots for better illustration purposes. Note that the half channel section has been further included for completeness:



(a) Streamwise velocity

(b) Spanwise velocity



(c) Total energy

FIGURE 6.8: Compressible ramp initial condition contour plot

6.3.4 Grid

The grid for this case problem was created using the commercial grid generator program **Gridgen**[®]. Grid clustering was employed again for the same reasons of resolving the boundary layer. However note that in this case, clustering was also used at the corner section of the compression ramp in the streamwise direction as can be seen in Figure 6.9 below in order to be able to capture the complex physics expected in the region due to the shock-boundary layer interaction. The elliptic solver was run down to a precision of 10^{-07} in the residual in order to generate a sufficiently smooth grid.

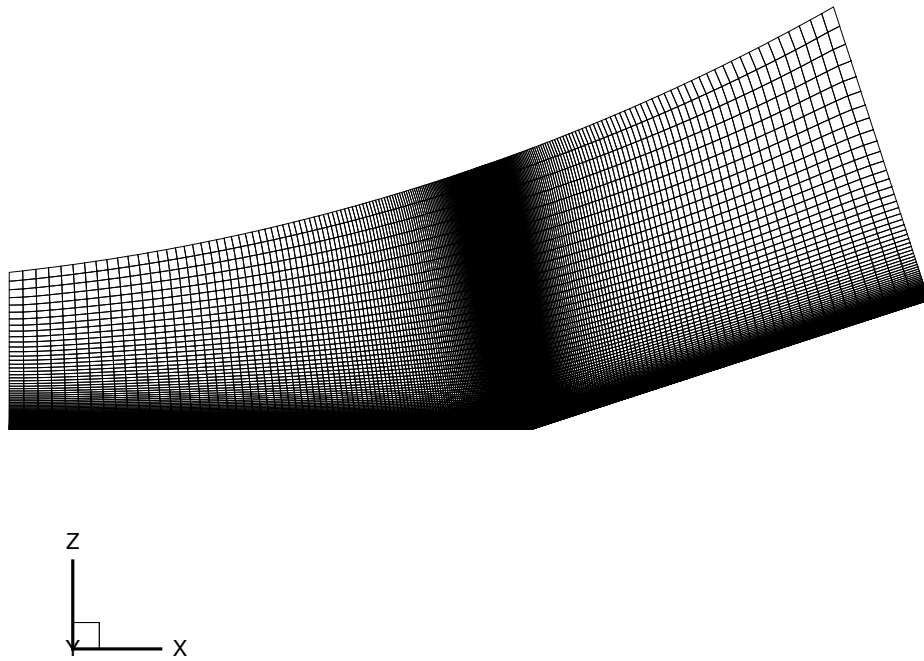


FIGURE 6.9: Compression ramp grid

The streamwise and wall normal clustering distribution is as:

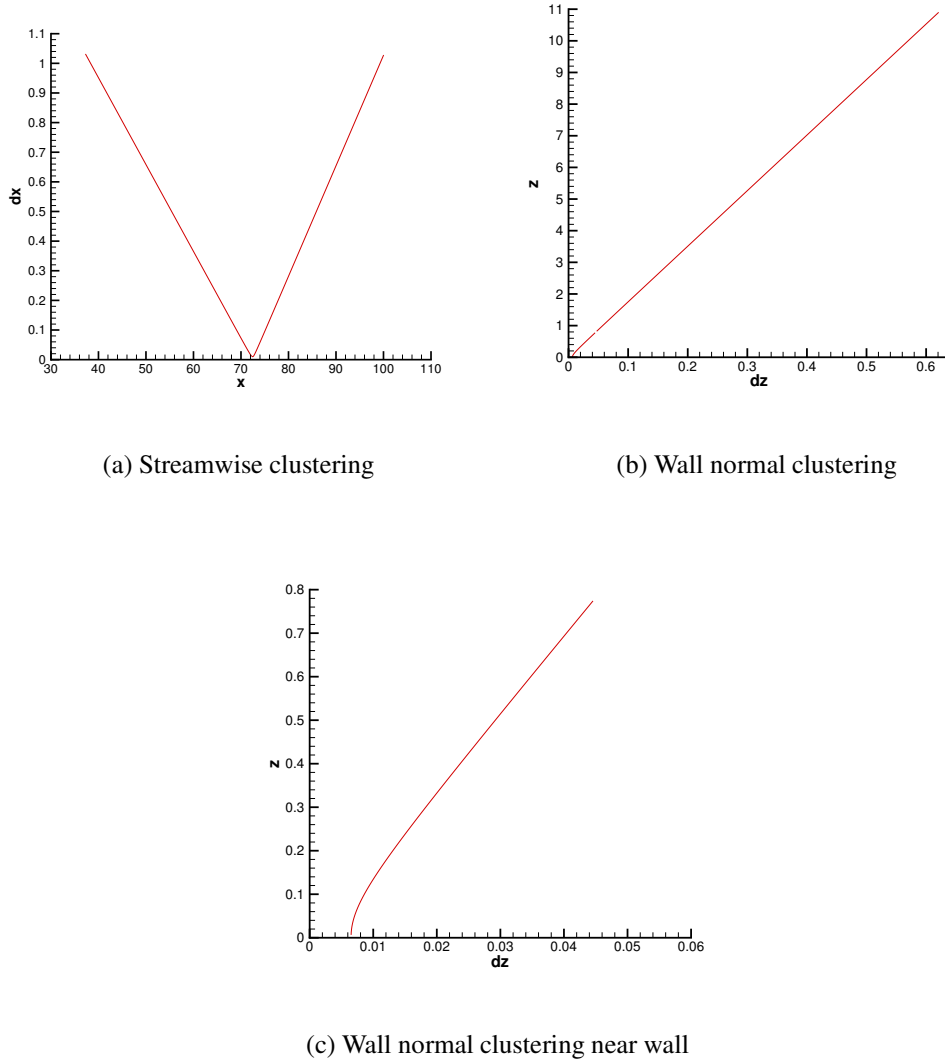


FIGURE 6.10: Clustering in compression ramp

The grid size was based on the dimensions of the grid used in [125]. It should be noted that no specifications of the grid clustering was given and therefore was clustered based on achieving a wall distance z^+ of one followed by the same distance in the streamwise direction in the ramp corner for unstretched cells. Thus the grid created does not necessarily reflect the same grid used in [125]. Note that from literature, the grids used for this particular case amount to three, one for DNS and two for LES as seen above in Table 6.2.1. Specifically the number of points used in [124] amount to 5,516,181 points, that is about 40% the size of the DNS simulation of [121, 122] with 14,400,000 points. The

other LES investigation of [125] totalled to 942,214 points at 6.5% of DNS [121, 122].

It is evident that the number of points employed in the two LES papers differ significantly. The LES of [124] used a 5.8 times larger grid compare to the one employed in [125]. Due to the huge difference in the total number of points and thus the computational expense, the grid used in [125] was selected since initially it can be used as a development platform for the particular investigation.

Regarding the half channel section, the spanwise and wall normal grid size and spacing is used. For the streamwise direction, the same number of points were taken as in the section of the ramp domain starting from the inlet and leading to the ramp corner which is also in dimensions of the same length. However in the half channel no corner exists and therefore no streamwise clustering was used. This results in a grid of size $186 \times 91 \times 31$, amounting to a total number of points of 524,706.

6.4 Results and Discussion

In this section the results obtained for the compression ramp are presented. The first parameter to compare against other simulations for the exact same compression ramp configuration (DNS [121, 122], LES [126]) are the velocity profiles. These are obtained at ten different stations in the ramp section along the streamwise direction as shown in Figure 6.11 and compared with those obtained by the DNS simulations of [121, 122]. Then the coefficient of friction C_f is used to observe features such as separation bubble size, shock strength and location and obviously near wall turbulent boundary layer capture. This is then followed by a presentation of iso-surfaces for various flowfield variables for the best developed case including Schlieren ($\nabla\rho$) snapshots of the flow. Since none of the experimental compression ramp literature includes a case with the same set-up, no comparisons against any has been made.

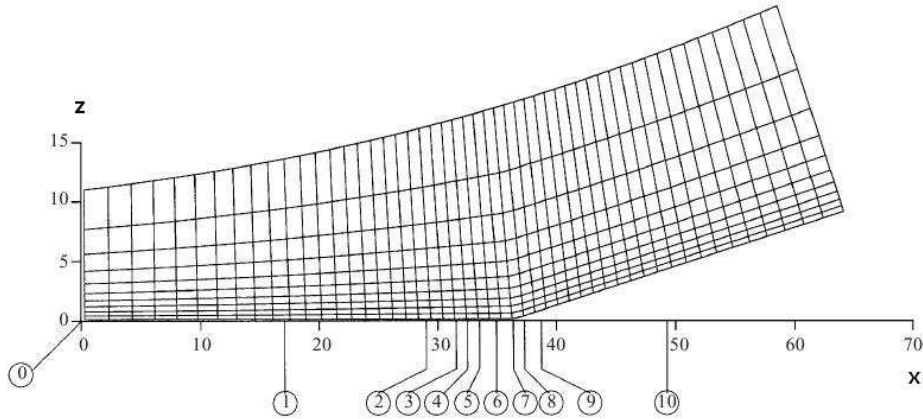


FIGURE 6.11: Compression ramp statistics stations

It is worth mentioning at this point that a solution was not possible to obtain with WENO 9th order due to the presence of the multiple shock wave structure near and around the shock-bubble interaction region. This, coupled with the fact that WENO 9th order requires a large stencil leads to an unphysical solution. In [127] it was observed that when high-order WENO reconstruction is based on the conservative variables, it leads to the appearance of an excessive amount of unphysical oscillations in the solution between the sharp discontinuities.

6.4.1 Half Channel Upper Boundary Condition

Here the boundary conditions applicable to the upper section in the wall normal direction of the half-channel domain are investigated in order to determine their suitability.

Supersonic Outflow

The implementation of the outflow boundary condition is a good example of a boundary condition being from a physical point of view correct but due to numerical 'details' developing an unphysical solution. An iso-contour slice of the half channel section can be seen below in Figure 6.12. Naturally the flow should have been reaching its freestream properties as it approached the upper boundary, however this was not the case here. The shock formations that formed originates due to the linear nature of extrapolation used for the supersonic outflow condition in conjunction with the fact that the flow is not actually 'exiting' the domain in that direction but is rather in a shear to the boundary.

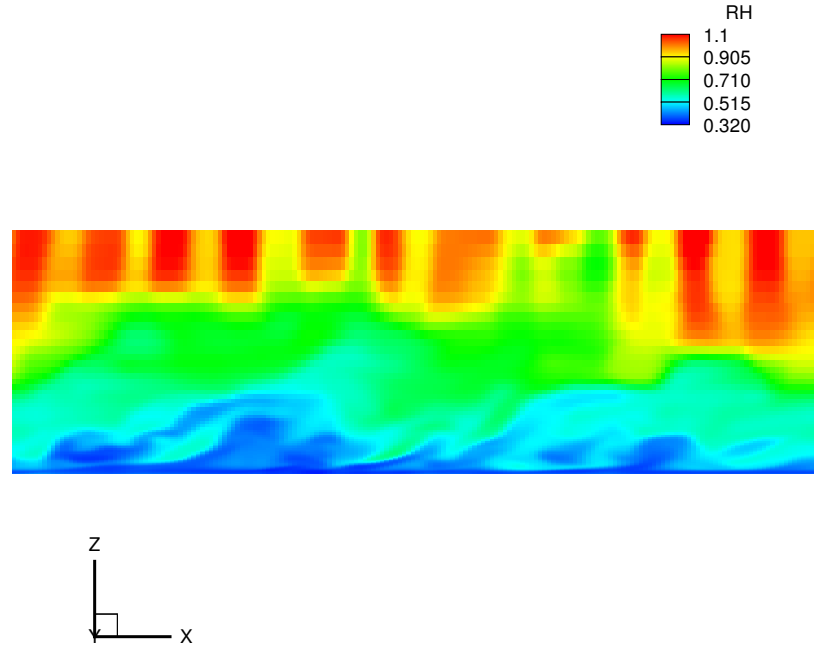


FIGURE 6.12: Contours of density in half channel outflow boundary condition

The linear extrapolation is an assumption that the flow varies near the boundary where the outflow is used by some linear gradient. However this is not always the fact especially for turbulent flows. Furthermore the fact that the grid is coarse in the upper region due to wall clustering only helps in increasing the gradient error, since the larger the distance, the less likely that the flow will vary in a linear manner. A graph of the wall normal velocity against the half-channel height below in Figure 6.13, shows how the flow actually behaves in a more curve-like fashion.

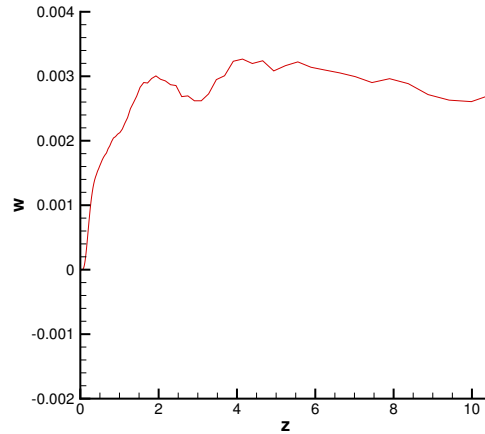


FIGURE 6.13: Wall normal velocity profile in half-channel using outflow BC

However the shock pattern would still not have occurred if it was not for the fact that the flow is in shear to the outflow BC. The linear errors of the supersonic BC 'bounce' back into the flow. At this point, the shear flow coupled with the periodic boundary condition in the streamwise direction, 'store' the error and as a result accumulates in time. Eventually an unusual shock wave pattern occurs resulting in the simulation stopping due to some non-realistic flowfield variable being obtained either as a zero density or negative total energy.

Also, the supersonic outflow boundary condition can be regarded as a relatively 'weak' boundary condition since it 'relaxes' the conditions required to be met at the boundary. On the other hand, a boundary condition like farfield or symmetry require a stringer condition to be met. In this regard, either could avoid the flow in developing the numerical artifacts by enforcing a smoother velocity distribution. However, a LES simulation is not guaranteed to capture the boundary layer correctly and therefore disturbances could accumulate by reflecting off the constant properties prescribed and thus leading to an incorrect flowfield. On the other hand, the symmetry condition is such that any perturbations (whether physical or numerical) will be cancelled (nullified) by symmetry. Though at first this may sound as an unphysical boundary condition for this case, it does however guarantee a smooth flow near the upper boundary such as it should in the freestream. For this reason the symmetry condition was selected as the upper boundary condition for the half-channel domain.

Symmetry

The symmetry boundary condition did not produce any unphysical flow structure as in the case of the supersonic outflow throughout the entire run time as can be seen in Figure 6.14. However it is also made evident that a larger part of the flow is of a higher density. This shows that the symmetry condition acts in a compressive manner due to the symmetry condition imposed to the wall normal velocity component which through cancelling out the vertical perturbation, it results in a high compressed flow-strip from the vertical perturbations being generated near the wall. It should be noted that the better the boundary layer is captured numerically, the less the resulting compressive effect near the upper symmetry boundary condition will be.

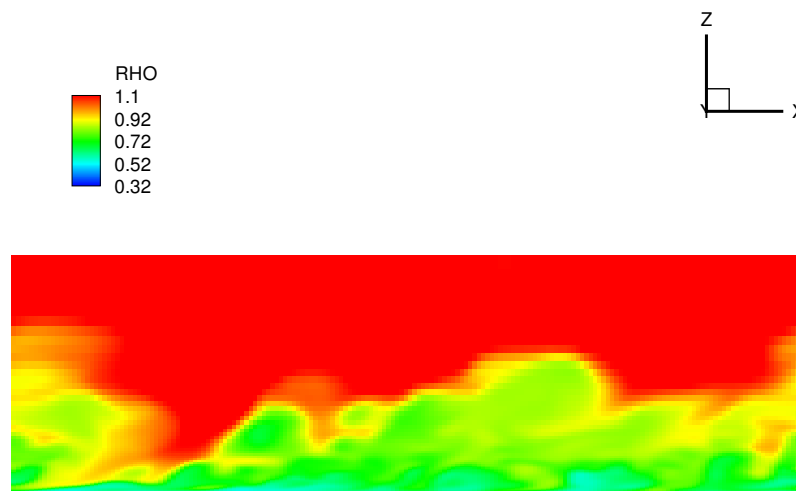


FIGURE 6.14: Contours of density in half channel symmetry boundary condition

This results in a thinner boundary layer as well, evident of the smaller low density (blue colour contours) area when comparing Figure 6.14 to Figure 6.12. The streamwise profile obtained in the half-channel section can be compared to that obtained using DNS on station 1 which is still relatively close to the inlet and should retain the same profile. Since MC proved the best second order limiter, it was applied initially for this case too.

As can be seen in Figure 6.15, the velocity profiles are in relatively good agreement near the wall with a deviation in the profiles occurring at the half-height.

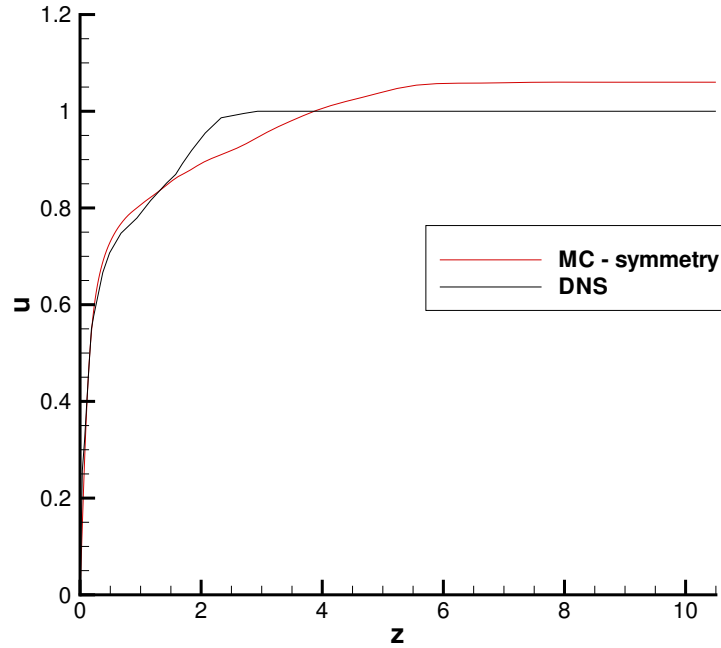
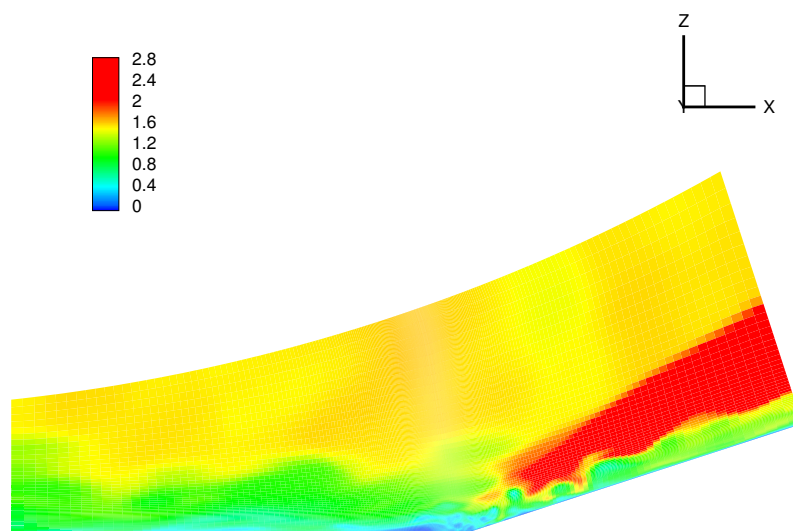


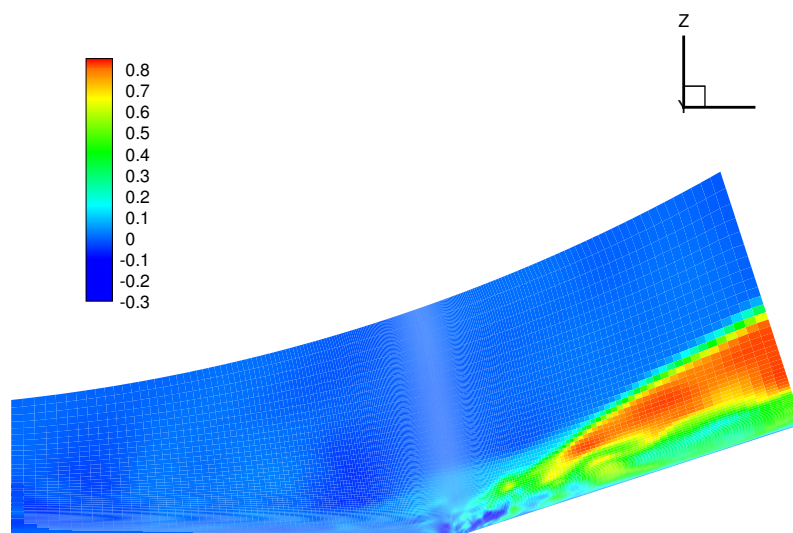
FIGURE 6.15: Streamwise velocity profile at ramp inlet

6.4.2 Flow Development & Characterisation

In this section a number of iso-contours of flowfield properties obtained from the numerical simulations are presented. In Figure 6.16 the streamwise and wall normal velocity contours are given. In Figure 6.16(a), one may observe the small dark blue region in the ramp corner depicting the presence of the separation bubble. One would expect to see a shock forming right over the bubble, however the contour level value range does not allow for a clear view due to the larger values of streamwise and wall normal velocities obtained further down the shock.



(a) Streamwise velocity



(b) Wall normal velocity

FIGURE 6.16: Contours depicting flowfield

Therefore it is hard to tell the structure of the flow at and around the ramp corner, let alone of the existence of any kind of shock-boundary layer interactions. Taking advantage of the fact that a shock wave is actually a compression wave that increases the density across a small region, a density gradient ($\nabla\rho$) contour plot should be able to 'uncover' the ramp corner's physics.

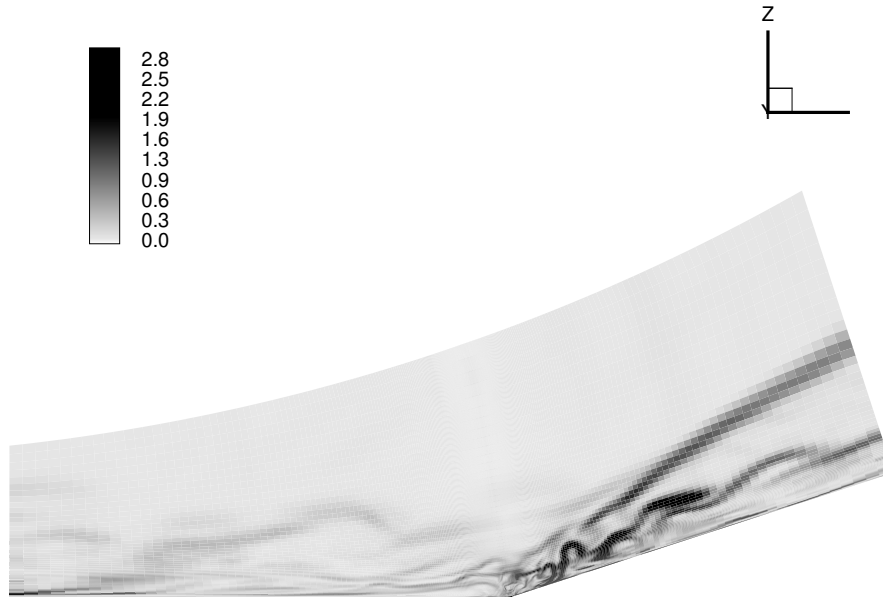


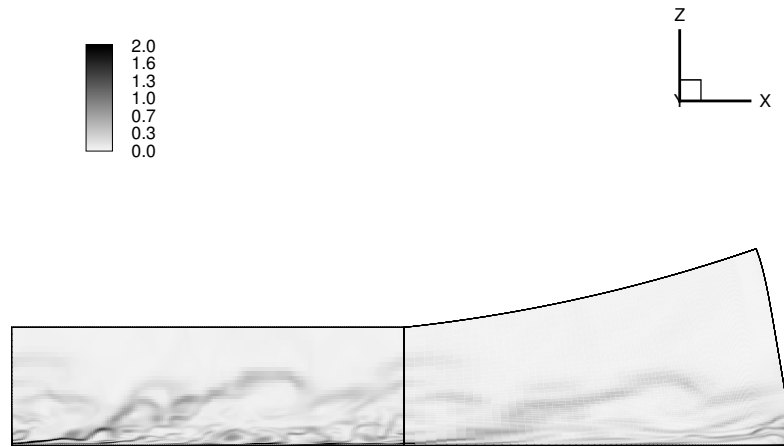
FIGURE 6.17: Schlieren-like contour plot depicting shock formation near the ramp corner

From Figure 6.17, the complex flow-structures located at the compression ramp corner are now revealed. As in the LES of [125], the large scale behaviour across the interaction is similar to that obtained in DNS [121, 122]. Though the shock foot observed in Figure 6.17 is not present in the DNS simulation, it is clearly visible in LES. The shock foot is at the origin of a high density-gradient interface starting from the boundary layer edge just before the ramp corner and extending downstream. Shortly after, the main shock wave body forms, propagating downstream with strong vortical features below it originating from its interaction with the separation bubble at the ramp corner.

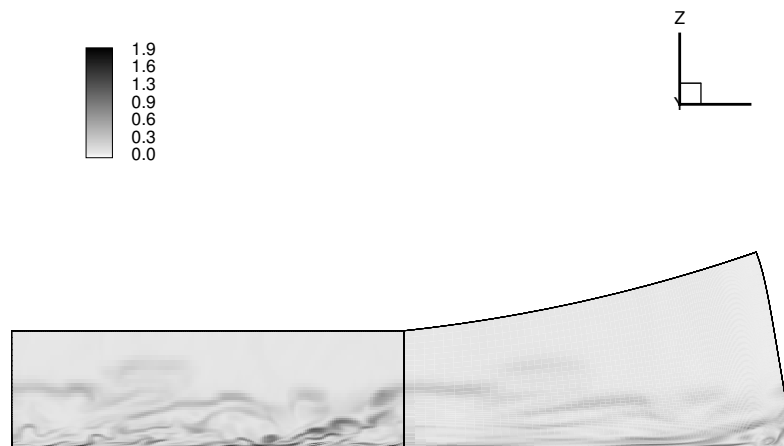
The thin elongated strips of density gradient prior to the shock are a clear indication

of the effect the grid clustering had. To get a better understanding as to how this happens, a couple of contour plots are made depicting the density gradient again but only for the domain comprising of the half-channel and the compression ramp section up to the corner point Figure 6.18. An interface line is drawn in the domain depicting the contact surface between the inlet and ramp section so that the progressive loss of turbulent scales can be noticed as the flow transfers from one domain to the next.

It should be noted that the limiter used for reconstruction in the half channel section for either case presented here was MC. This was not the case for the compression ramp section for which different limiters were employed, namely VL and MC. When comparing the MC against the VL limiter in the Schlieren-like instantaneous streamwise slices of Figure 6.18, it can be noticed that the thin elongated streamwise streaks appear to be of a more defined appearance for the former. It is clear that MC has a finer and better ordered turbulent structure. In either case though, the 'blurring' of the incoming flowfield, else diffusion of the solution, in the ramp's inlet section is clearly visible and explains the slightly poorer results obtained for the coefficient of friction in the pre-shock section.



(a) MC



(b) VL

FIGURE 6.18: Schlieren ($\nabla\rho$) like contours depicting flowfield for corresponding limiter in half-channel ramp sections

6.4.3 Momentum Profiles

The mean contravariant streamwise $\langle \overline{\rho u_c} \rangle$ and wall normal $\langle \overline{\rho w_c} \rangle$ momentum profiles obtained with the VL and MC limiter using a symmetry-outflow BC combination for the half-channel and compression ramp upper boundaries respectively are shown. Angles $\langle \rangle$ indicate statistical averages with the overbar denoting ensemble average and contravariant momentums are referred to the Cartesian momentums through

$$\rho u_c = \frac{\rho u n_x^{\perp yz} + \rho w n_z^{\perp yz}}{\sqrt{(n_x^{\perp yz})^2 + (n_z^{\perp yz})^2}}$$

and

$$\rho w_c = \frac{\rho u n_x^{\perp xy} + \rho w n_z^{\perp xy}}{\sqrt{(n_x^{\perp xy})^2 + (n_z^{\perp xy})^2}}$$

where the $\perp$ identifies normal to a cell face area projection in the superscript plane in the subscript direction.

The profiles are obtained at a total of ten stations along the ramp as shown in Figure 6.11 and are presented in an increasing index number, hence in a downstream fashion. By contravariant components of momentum, the parallel component of momentum to the wall surface is meant.

First is station one. Here a relatively good profile for both streamwise and wall normal momentums against those obtained in DNS proves that the ILES simulation conducted in the half-channel section sufficiently resolved the presence of most turbulent structures. The slight deviation noticed in the contravariant wall normal momentum as moving towards the upper boundary in Figure 6.19 - 6.28 occurs for two reasons. First, the grid is much coarser in the upper region and therefore it is expected not to give as good results as in the near wall region. Secondly, the outflow boundary condition allows the flow to obtain a slightly higher momentum compare to what the farfield has thus resulting in a higher value too.

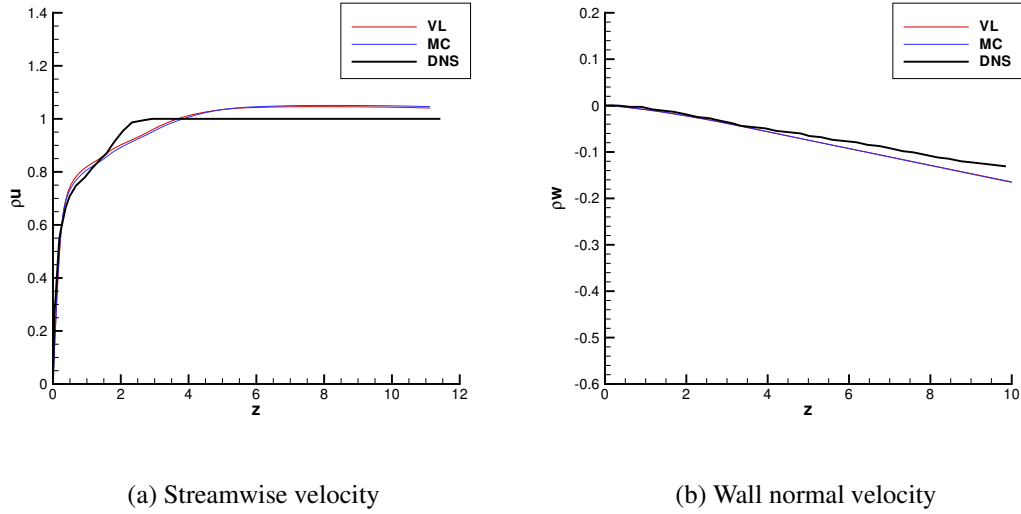
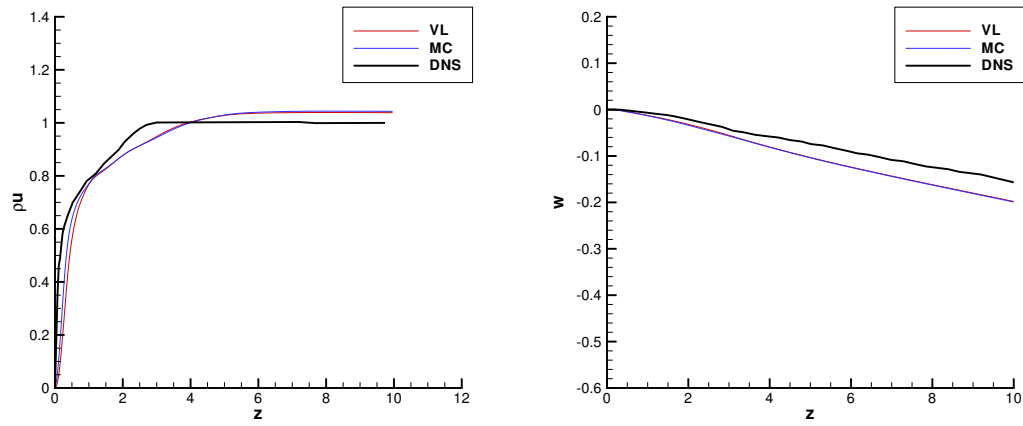


FIGURE 6.19: Station 1 velocity profiles

In stations 2 to 6, it is evident that the profile of the contravariant streamwise momentum near the wall progressively deteriorates. Although the clustering in the wall normal direction remained the same, the cells near the ramp inlet became stretched due to the clustering in the streamwise direction. This streamwise stretching effect on the cells in the ramp's inlet section results in the loss of the smaller, finer turbulent scales incoming from the half-channel section.

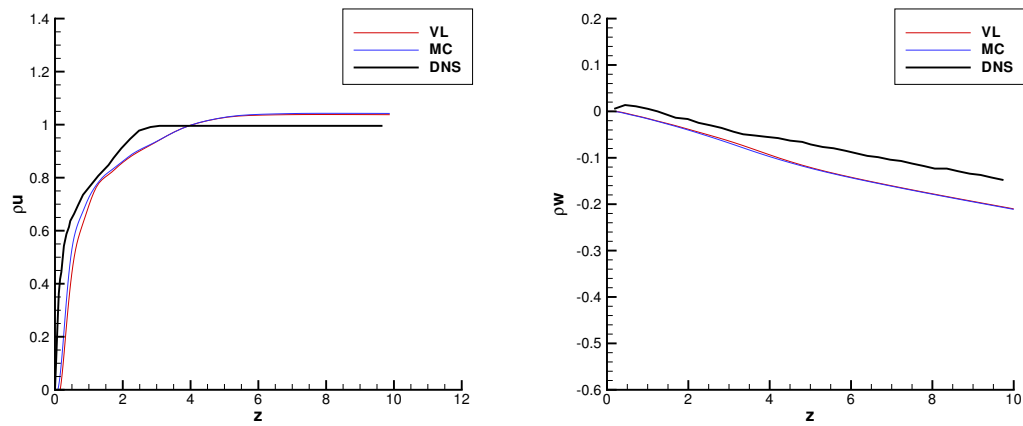
Further it is clear that the bubble forms relatively late compare to the DNS. This can be noticed by the wall normal momentum, where a 'bump' in the profile for DNS occurs from station 4 onwards. This does not occur in the results from the ILES computations until station 7. The reason for this again, is the outflow boundary condition that 'relaxes' the momentum in the wall normal direction by allowing oscillations to 'escape' through the boundary. However the general profile trends are still in good agreement to those of DNS.



(a) Streamwise velocity

(b) Wall normal velocity

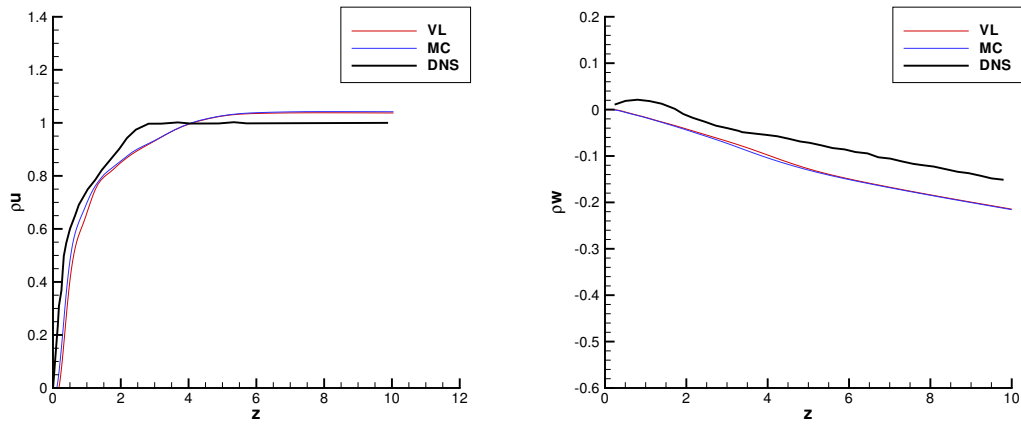
FIGURE 6.20: Station 2 velocity profiles



(a) Streamwise velocity

(b) Wall normal velocity

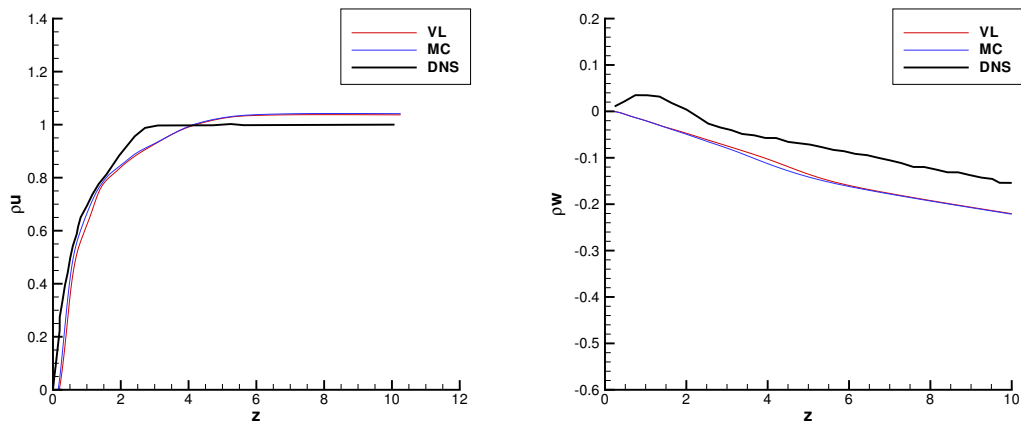
FIGURE 6.21: Station 3 velocity profiles



(a) Streamwise velocity

(b) Wall normal velocity

FIGURE 6.22: Station 4 velocity profiles



(a) Streamwise velocity

(b) Wall normal velocity

FIGURE 6.23: Station 5 velocity profiles

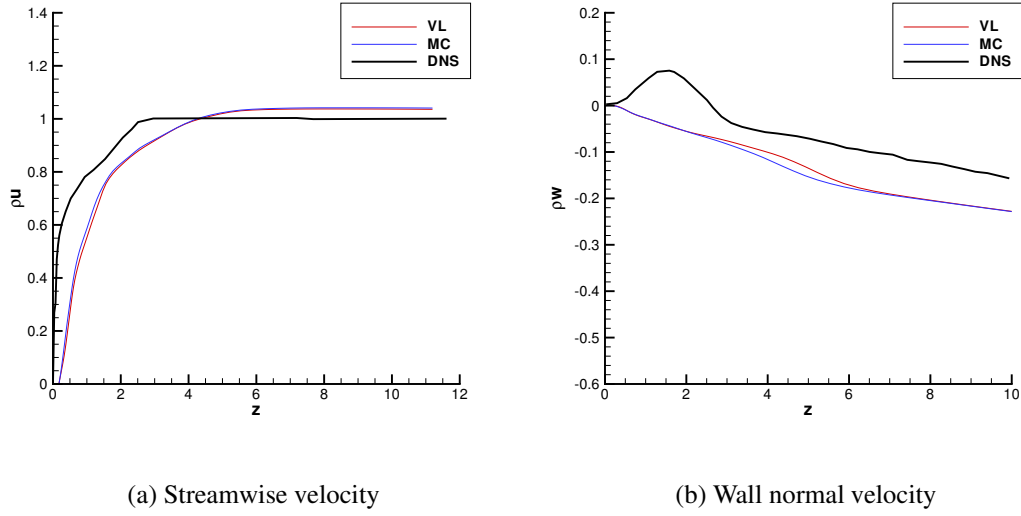


FIGURE 6.24: Station 6 velocity profiles

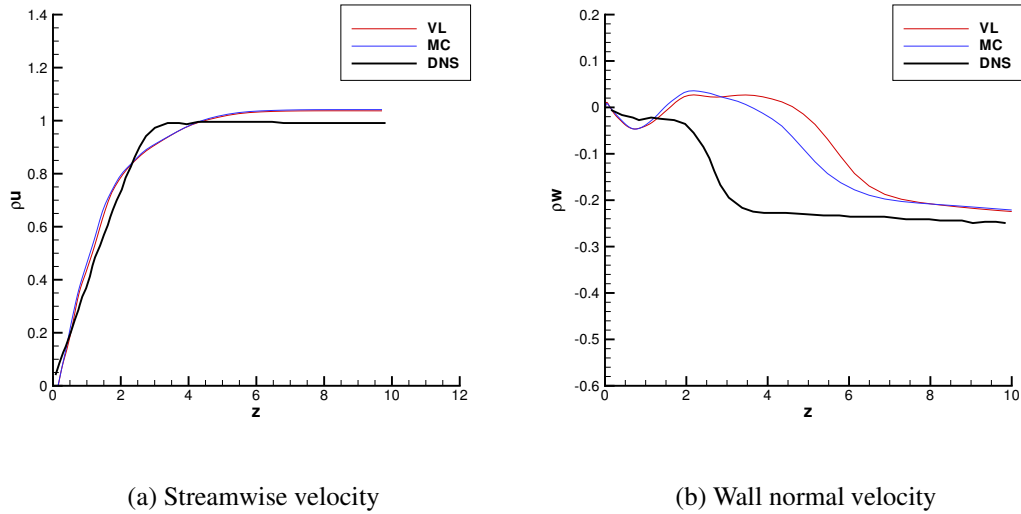


FIGURE 6.25: Station 7 velocity profiles

Stations 8 and after are located in the post-shock wave region of the domain. Here along with station 7 which is located where the shock wave starts to form, the streamwise momentum profiles align themselves sufficiently well to the DNS results. This shows that the clustering used for the streamwise and wall normal direction managed to resolve

the flow again, however the more curve-like wall normal momentum is due again to the supersonic outflow condition. This is profoundly evident from stations 7 and onwards especially in regards to the wall normal momentum, were a farfield boundary condition enforcing the freestream values has a much stronger impact on the profile as can be seen by the larger constant freestream values of momentum at and near the upper boundary.

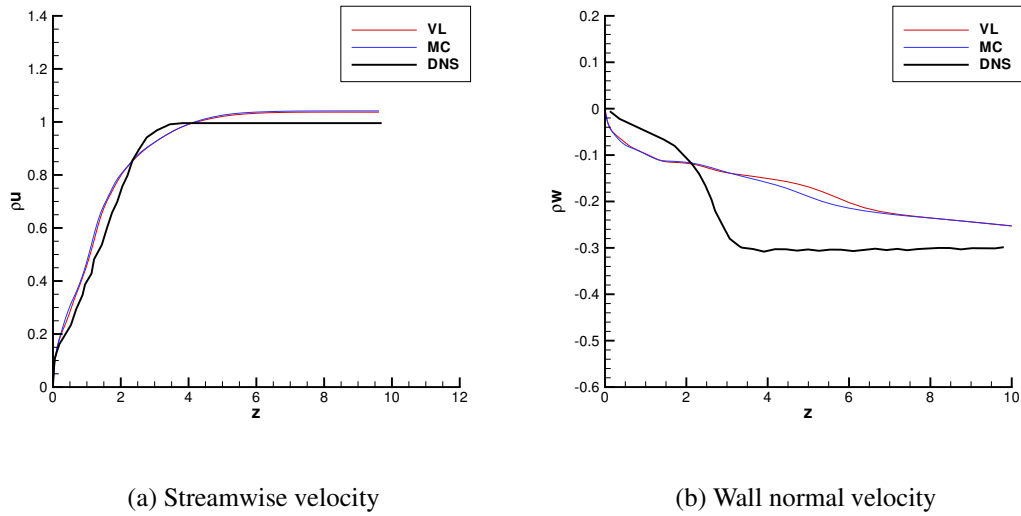


FIGURE 6.26: Station 8 velocity profiles

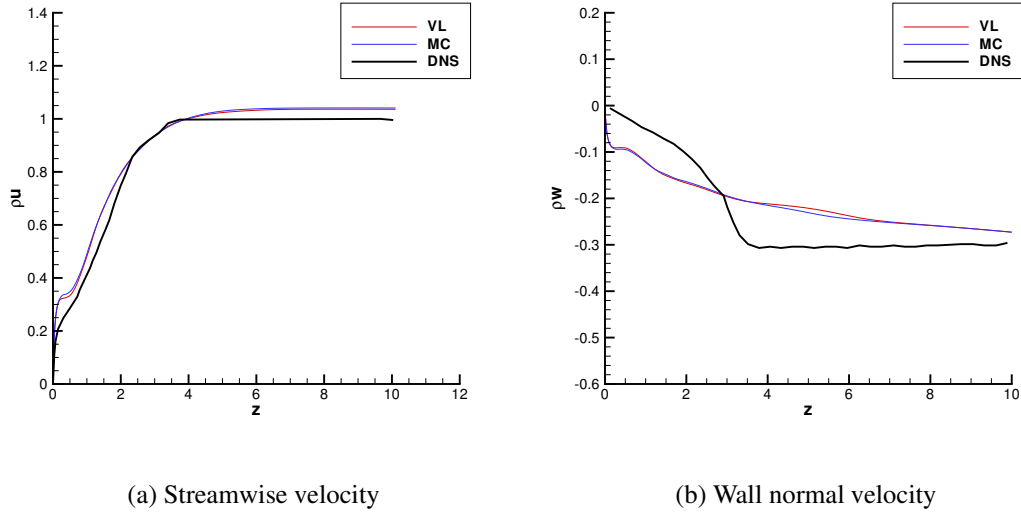


FIGURE 6.27: Station 9 velocity profiles

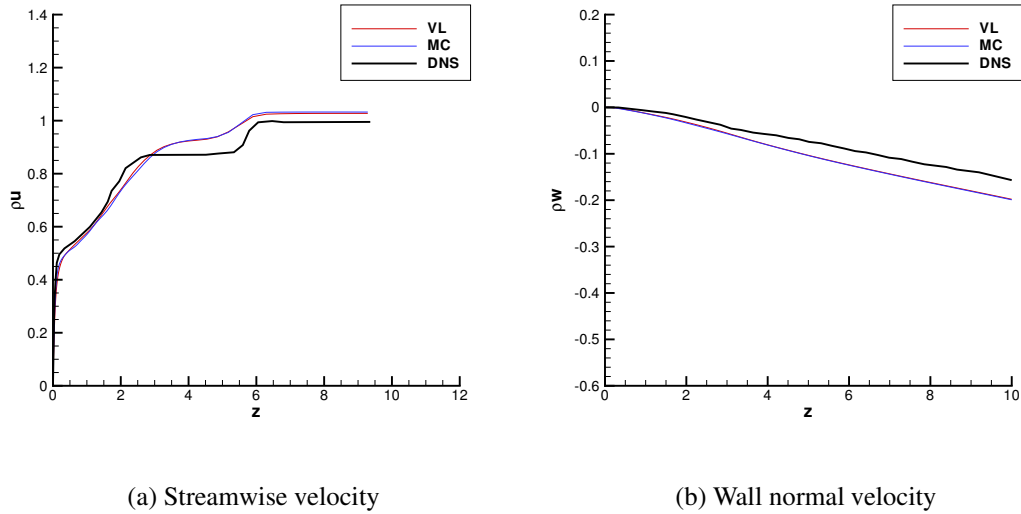


FIGURE 6.28: Station 10 velocity profiles

6.4.4 Coefficient of Friction

The coefficient of friction is one of the hardest coefficients to obtain correctly in compressible ramp flows as also admitted in [125]. The reason for this is obviously the fact

that a number of key flow features need to be captured correctly. Enough emphases on the importance of the grid in this case cannot be stressed out especially when all computations are conducted within the (I)LES framework. Grid clustering needs to be employed along the solid wall in order to adequately capture the boundary layer as well as the shock-boundary layer interaction at the corner point of the ramp which further requires clustering in the streamwise direction as well.

Apart from the ramp section however there is the half channel domain to be concerned about. Justifiably, it can be regarded just as important since poor results here can lead to even worse results in the ramp section. For example a poor turbulent inflow from the half channel domain can lead to a thicker boundary layer which immediately effects the skin friction obtained. Further, this can lead to a larger separation bubble, effecting not only the friction coefficient but also the shock formation and downstream flow as well. By comparing the coefficient of friction in Figure 6.29 at the inlet, it can be seen that the value obtained using the MC limiter was of an acceptable magnitude.

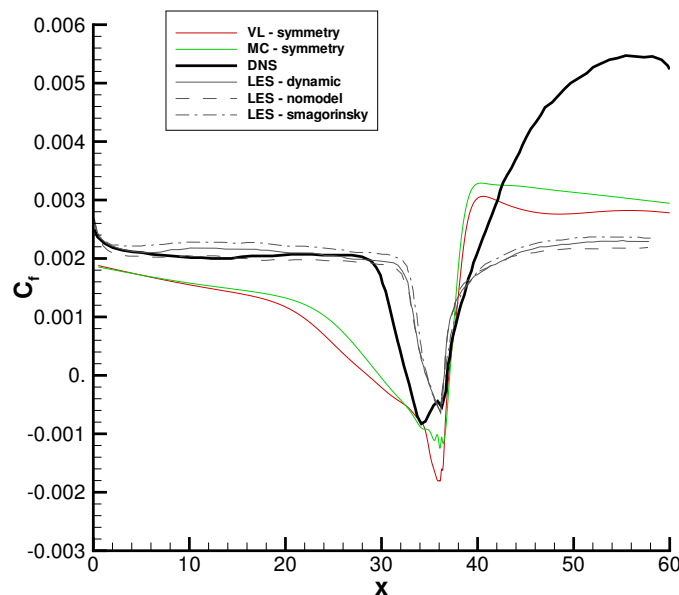


FIGURE 6.29: Coefficient of friction along solid wall in streamwise direction

The gradual decrease in the coefficient of friction from the ramp inlet leading to the

ramp corner at about position $x \approx 36.2$ is due to, as discussed when analysing the contravariant momentum profiles obtained, the clustering of the grid in the streamwise direction resulting in a coarse grid in the downstream direction. Thus there is a gradual 'loss' of quality in turbulence resolution as the flow passes through the coarser mesh at the ramp inlet, eventually leading to a thicker boundary layer and hence a decrease in the near wall velocity.

However the shock position is well captured as noticed by the bottom peak of the coefficient of friction with the difference of magnitude explained by the thicker boundary layer as previously discussed. In this regards, MC performs relatively better in obtaining a slightly later 'drop-off' point indicating that a better estimation of the friction velocity is obtained as noticed for the fully developed turbulent channel flow. Even better, the MC limiter predicts a smoother and smaller negative overshoot of the coefficient of friction at the ramp corner where the shock-boundary layer interaction occurs compared to the VL limiter. In the recovery zone or post-shock wave region of the ramp, the coefficient of friction is well resolved and compare to the LES investigation of [126] gave much better results in all cases.

The primary reason for the discrepancies observed in the pre-shock region is that the grid used in [126] was considerably finer. Furthermore it had better clustering in the streamwise direction in the pre-shock region in order to maintain the inflow turbulence at an acceptable level (see Section 6.3.4). In the case reported here, finer clustering is maintained in the post-shock region leading to better recovery of the coefficient of friction at the expense of the pre-shock region.

7

Conclusion

The work completed in this thesis covered a wide range of flows, from the low Mach number incompressible to supersonic compressible wall bounded flows using high-resolution methods in the context of Implicit Large Eddy Simulations (ILES). The resulting findings and conclusions made will be presented in the following section followed by recommendations for future work that may help in obtaining a deeper understanding of the solutions and results provided by using high-resolution methods and their inherent turbulence modelling capability with the hope of further improving them.

7.1 Conclusion of Work

Simulations based on the compressible NSE equations using high-resolution methods were carried out. No SGS turbulence model was used as the aim of the investigation was to examine the ILES ability to successfully model the dissipation of the SGS in Mach number flows ranging from low subsonic incompressible values of $M = 0.2$ to supersonic ones of $M = 3.0$. The former value was used in a fully developed turbulent channel flow for which no current compressible ILES investigation has been conducted.

It was demonstrated that a novel low Mach number treatment (LMNT) approach applied to reconstructed values obtained from the limiters can yield accurate comparisons with the DNS results on relatively coarse grids while at the same time improving results on the finer meshes considerably. From the observations made on different grids, a coarse grid may produce relatively bad results with the second order scheme, however application of either higher order schemes or LMNT improves the results significantly. Application of LMNT to the MC limiter, for example, can yield coarse grid results similar to those obtained on a grid of twice the size without LMNT. It should be noticed that the increase of the computational time per time step due to the application of LMNT is negligible. At the same time decreased dissipation of LMNT leads to much faster flow development and transition to turbulence which overall results in much smaller computational times.

However the investigation of the LMNT highlighted a potential issue with ILES methods. In the past ILES, and MILES in particular, was considered to be quite dissipative, and the main direction of research was associated with the application of increasingly high order methods. Application of LMNT to WENO 9th order revealed that the opposite trend can be observed. Insufficient dissipation in this case can lead to a converged, numerically stable solution which accurately predicts flow averages however yields unphysical behaviour of Reynolds stresses and higher order statistics. Which highlights that the main challenge of ILES is to provide not low, but rather adequate dissipation.

The second case investigated in this thesis was a supersonic compression ramp. This case was selected in order not only to investigate the numerical abilities of high-resolution methods and ILES in the supersonic regime but also their ability to deal with a variety of complex flow phenomena such as supersonic turbulent boundary layer, shock waves, boundary layer separation and shock-boundary layer interaction. In order to obtain the turbulent flow, the channel flow case above was taken advantage of and modified to the specific flow problem. Thus a novel method of obtaining the turbulent inlet boundary condition for the ramp was proposed, which leads to time-accurate turbulent inflow condition throughout the simulation and does not require data from DNS computations of a flat plate, which has been the preferred approach up to date.

The application of LMNT in this context has not been investigated due to the main part of the flow being supersonic. A steady drop in the coefficient of friction observed in the pre-shock section was mainly attributed to the streamwise grid resolution employed. However strong clustering in the post-shock section resulted in the accurate prediction of the position of the shock as well as some of the major flow field characteristics in

this region, such as the separation bubble and shock-foot. Further, better recovery of the coefficient of friction was obtained in the post-shock ramp section in comparison with classical LES investigations reported to date. The contravariant streamwise momentum profiles obtained at a number of stations at progressive streamwise locations were all comparable to the ones obtained in the DNS simulations. The same applied to most of the contravariant wall normal momentum profiles with a few exceptions. However these still withheld the general DNS profile variation.

7.2 Future Work

Building on the conclusions of this study, further analysis of the LMNT behaviour based on the energy cascade analysis and energy spectrum seems to be necessary, especially for the 9th order WENO scheme so that the underlining reasons of the overprediction of turbulence intensity are clarified. This could help identify at which turbulent scales less dissipation is introduced when compared to the theoretical Kolmogorov energy cascade and why it mainly affects the wall normal velocity component. This can be interestingly followed by the application of a MUSCL 7th and/or 9th order scheme applied along with LMNT to investigate whether the same turbulence overprediction occurs with higher order reconstruction methods as with WENO 9th. This research can ultimately lead to the development of a turbulence-resolving limiter which ensures that adequate numerical dissipation is provided which is capable of mimicking sub-grid scales behaviour.

For the compression ramp, the implications of using farfield boundary condition at the upper section requires further investigation. While there is little point in increasing the overall grid size, especially taking into account that the main benefit of LES in comparison with DNS is lower overall computational requirements, a more carefull design of the clustering and point allocation can be looked into in order provide an optimal result for a given grid size. Additionally, the application of 9th order WENO in the characteristic form can be investigated, particularly since some authors suggest that in this formulation it can handle multiple shock interfaces better than the conservative form employed in this thesis. As a final proposal for future work, the application of LMNT to the subsonic region of the flow, mainly consisting of the subsonic part of the turbulent boundary layer, and it's possible effect on the resolution of the shock-boundary layer interaction need to be examined.

Appendices and References

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Appendix A

A.1 Some Noteworthy Relationships

For the convenience of the reader, some core mathematical relationships are presented which are used throughout the thesis.

A.1.1 Line Integrals

A vector field is considered in the cartesian frame of reference so

$$\vec{\alpha} = \vec{\alpha}(x, y, z)$$

Furthermore, a curve C is considered which connects two points a and b as shown in Figure A.1(a). If ds is an elemental length of the curve and $\vec{n}$ is a unit vector tangent to the curve, the vector can be defined as $d\vec{s} = \vec{n}ds$. Hence the line integral of $\vec{\alpha}$ along curve C from points a to b is:

$$\int_a^b \vec{\alpha} \cdot d\vec{s}$$

If the curve C is closed, as shown in Figure A.1(b), then the line is given by

$$\oint_C \vec{\alpha} \cdot d\mathbf{s}$$

where the counter-clockwise direction around C is taken as the positive direction so

$$\oint_C \vec{\alpha} \cdot d\mathbf{s} = \oint_C \vec{\alpha} \cdot d\mathbf{s}$$

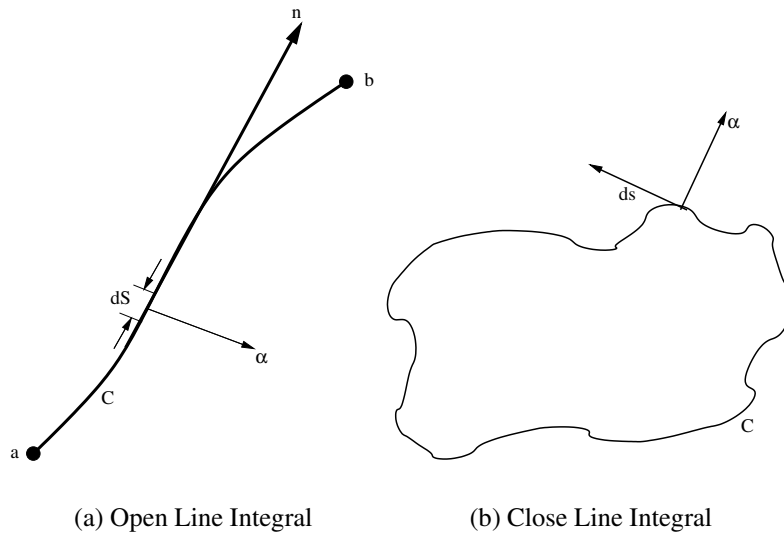


FIGURE A.1: Line Integrals

A.1.2 Surface Integral

An open surface A bounded by a closed curve C is considered as shown in Fig A.2. If dA is an elemental area of the surface at point k and $\vec{n}$ is the unit vector normal to the surface then the vector elemental area $d\mathbf{A}$ can be defined as $d\mathbf{A} = \vec{n}dA$.

$$\begin{aligned}
\iint_A x dA &= \text{surface integral of a scalar } x \text{ over the open surface } A \text{ (result is scalar)} \\
\iint_A \vec{a} \cdot d\mathbf{A} &= \text{surface integral of a vector } \vec{a} \text{ over the open surface } A \text{ (result is scalar)} \\
\iint_A \vec{a} \times d\mathbf{A} &= \text{surface integral of a vector } \vec{a} \text{ over the open surface } A \text{ (result is vector)}
\end{aligned}$$

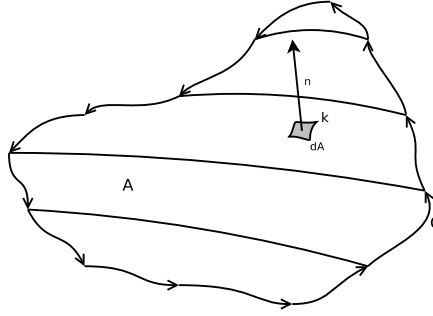


FIGURE A.2: Surface Integral

The surface integral over the surface A can be defined in terms of $d\mathbf{A}$ in the following three ways: If the surface A is closed (as that of a sphere or cube) and $\vec{n}$ points out along the normal to the surface as shown in Fig 2.1, the surface integrals are respectively to above,

$$\begin{aligned}
\oiint_A x dA \\
\oiint_A \vec{a} \cdot d\mathbf{A} \\
\oiint_A \vec{a} \times d\mathbf{A}
\end{aligned}$$

A.1.3 Volume Integral

If a Control Volume, CV, in space is considered and x is a scalar field in this space, then the volume integral over the volume V of the quantity k is written as

$$\iiint_V x dV = \text{volume integral of scalar } x \text{ over the CV (result is scalar)}$$

The corresponding volume integral for a vector field $\vec{\alpha}$ over the CV is

$$\iiint_V \vec{\alpha} dV = \text{volume integral of vector } \vec{\alpha} \text{ over the CV (result is vector)}$$

A.1.4 Relation Between Line, Surface and Volume Integrals

Consider an open area A bounded by the close curve C , as shown in Fig A.2 and let $\vec{\alpha}$ be a vector field. The line integral of $\vec{\alpha}$ over C is related to the surface integral of $\vec{\alpha}$ over A by *Stokes theorem*:

$$\oint_C \vec{\alpha} \cdot d\mathbf{s} = \iint_A (\nabla \times \vec{\alpha}) \cdot d\mathbf{A} \quad (\text{A.1})$$

Now consider the same volume V enclosed by the closed surface A , as as shown in Fig 2.1. The surface and volume integrals of the vector field $\vec{\alpha}$ are related through the *divergence theorem*, also known as *Gauss' theorem*:

$$\oiint_A \vec{\alpha} \cdot d\mathbf{A} = \iiint_V (\nabla \cdot \vec{\alpha}) dV \quad (\text{A.2})$$

If χ represents a scalar field, a vector relationship analogous to Eq A.2 is given by the *gradient theorem*:

$$\oiint_A \chi d\mathbf{A} = \iiint_V \nabla \chi dV \quad (\text{A.3})$$

A.2 Thermal Conductivity

The thermal conductivity k is widely accepted to be composed of the sum of two parts, a laminar and a turbulent component. This is done in order to enable mechanisms of turbulent transport to be correctly accounted for. Thus:

$$k = k_l + k_t \quad (\text{A.4})$$

where k_l is the laminar component and k_t is the turbulent component. Note that in the case of ILES where no turbulence model is used explicitly, the turbulent thermal conductivity is neglected and therefore equals zero $k_t = 0$. In order to account for the laminar and turbulent components of the thermal conductivity, the Prandtl Number is also expressed

in the form of the two same components. Furthermore, since the ratio c_p/Pr is approximately constant for most gases, the thermal conductivity k may also be calculated by

$$k = \frac{\mu c_p}{Pr_l} + \frac{\mu c_p}{Pr_t} \quad (\text{A.5})$$

For air, the value of the laminar Prandtl Number Pr_l is given as 0.72 while its turbulent counterpart Pr_t as 0.9.

B

Appendix B

B.1 Differential Form of Conservation Equations

As already mentioned, the equations solved for simulating a flow are the NSE. In Section 2.1 the NSE were presented in integral form and in particular a complete formulation was derived, Eq. 2.13, in Section 2.4 . For a Newtonian viscous fluid they comprise of the continuity, momentum and energy equation and for an unsteady compressible 3-Dimensional viscous flow in conservation form are written as follows:

Continuity

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u_j) = 0 \quad (\text{B.1})$$

, u is the velocity, ρ is the density and t is the time.

Momentum

$$\frac{\partial \rho u_i}{\partial t} + \nabla \cdot (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \nabla \cdot (\tau_{x_i x_j}) \quad (\text{B.2})$$

For a Newtonian fluid, assuming Stokes Law of mono-atomic gases, the viscous stress $\tau_{x_i x_j}$ is given by

$$\tau_{x_i x_j} = 2\mu S_{x_i x_j}$$

and the trace-less viscous strain-rate tensor is defined as

$$S_{x_i x_j} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k}$$

, where δ_{ij} is the Kronecker delta (discrete version of the delta function) defined as:

$$\delta_{ij} = \begin{cases} 0, & \text{for } i \neq j \\ 1, & \text{for } i = j \end{cases}$$

Also $i, j = 1, 2, 3$ which correspond to the x, y, z directions respectively.

Energy

$$\begin{aligned} \frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho E u_j) &= -\nabla \cdot (p u_j) - \nabla \cdot (\rho \dot{q}_j) + \\ &\quad \nabla (u_i \tau_{x_j x_i}) \end{aligned} \quad (\text{B.3})$$

, where $\dot{q}$ is the heat flux:

$$\dot{q}_j = -\kappa \frac{\partial T}{\partial x_j}$$

and κ is the thermal conductivity coefficient.

B.2 Governing Equations in Vector Variable Form

It is possible to observe that the conservation form of the NSEs given in the previous subsection all have the same generic form, that of:

$$\frac{\partial U}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} = \frac{\partial R}{\partial x} + \frac{\partial S}{\partial y} + \frac{\partial L}{\partial z} \quad (\text{B.4})$$

, where U is the array of the conservative variables sometimes referred to as the solution vector. E, F and G are the the inviscid flux vectors whereas R, S, L are the viscous. Hence

considering Eqn. B.1 to B.3 the vector arrays of Eqn B.4 are:

$$\begin{aligned}
 U &= \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho \end{pmatrix}, \quad E = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho v u \\ \rho w u \\ (e + p) u \end{pmatrix}, \quad F = \begin{pmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ \rho w v \\ (e + p) v \end{pmatrix}, \quad G = \begin{pmatrix} \rho w \\ \rho u w \\ \rho v w \\ \rho w^2 + p \\ (e + p) w \end{pmatrix} \\
 R &= \begin{pmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xz} \\ u\tau_{xx} + v\tau_{xy} + w\tau_{xz} - \dot{q}_x \end{pmatrix}, \quad S = \begin{pmatrix} 0 \\ \tau_{yx} \\ \tau_{yy} \\ \tau_{yz} \\ u\tau_{yx} + v\tau_{yy} + w\tau_{yz} - \dot{q}_y \end{pmatrix} \\
 L &= \begin{pmatrix} 0 \\ \tau_{zx} \\ \tau_{zy} \\ \tau_{zz} \\ u\tau_{zx} + v\tau_{zy} + w\tau_{zz} - \dot{q}_z \end{pmatrix}.
 \end{aligned} \tag{B.5}$$

B.3 Curvilinear Transformation

Till now, the equations have remained in the Cartesian Coordinate system. Thus in order for Eq. B.4 to be applicable, the arrangement of the grid points would require to be of an orthogonal relationship and to be spaced equally along each axis, that is an uniform rectangular grid. While this does not cause a problem for simple geometries composing of straight and perpendicular lines (such as a channel flow), it can be for more complex geometries that have curved lines (such as airfoils). In those cases a non-uniform grid has to be used and therefore the NSEs as are in the form of Eq. B.4 will have to be recasted so as to be applicable on a transformed uniform rectangular grid. What must be done is to transform the partial differentials in Eq. B.4 from being differentiated with respect to the x, y, z Cartesian coordinates to being differentiated with respect to the curvilinear ξ, η, ζ coordinate system in such a way that the non-uniformly distributed grid points in the Cartesian co-ordinate system are uniformly distributed resulting in a rectangular grid. Therefore there exists a relationship between ξ, η, ζ and x, y, z capable of transforming the

grid from non-uniform to uniform rectangular and hence ξ, η, ζ are functions of x, y and z :

$$\begin{aligned}\xi &= \xi(x, y, z, t) \\ \eta &= \eta(x, y, z, t) \\ \zeta &= \zeta(x, y, z, t) \\ \tau &= \tau(t)\end{aligned} \quad (B.6)$$

Using these relationships yields:

$$\frac{\partial \widetilde{U}}{\partial \tau} + \frac{\partial \widetilde{E}}{\partial \xi} + \frac{\partial \widetilde{F}}{\partial \eta} + \frac{\partial \widetilde{G}}{\partial \zeta} = \frac{\partial \widetilde{R}}{\partial \xi} + \frac{\partial \widetilde{S}}{\partial \eta} + \frac{\partial \widetilde{L}}{\partial \zeta}, \quad (B.7)$$

where:

$$\begin{aligned}\widetilde{U} &= JU \\ \widetilde{E} &= J(E\xi_x + F\xi_y + G\xi_z) \\ \widetilde{F} &= J(E\eta_x + F\eta_y + G\eta_z) \\ \widetilde{G} &= J(E\zeta_x + F\zeta_y + G\zeta_z), \\ \widetilde{R} &= J(R\xi_x + S\xi_y + L\xi_z) \\ \widetilde{S} &= J(R\eta_x + S\eta_y + L\eta_z) \\ \widetilde{L} &= J(R\zeta_x + S\zeta_y + L\zeta_z)\end{aligned} \quad (B.8)$$

where J denotes the Jacobian determinant of the transformation of the NSEs from the Cartesian coordinates t, x, y, z system (computational plane) to the curvilinear coordinate system τ, ξ, η, ζ (physical plane):

$$J \equiv \frac{\partial(x, y, z)}{\partial(\xi, \eta, \zeta)} \equiv \begin{vmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{vmatrix}. \quad (B.9)$$

So the reduction of the NSEs to one equation capable of being used on a curvilinear grid has been achieved, thus helping to simplify the structure and logic of the CFD code. An example of the above procedure can be seen in Fig. B.1. The transformed grid is named the computational domain since all calculations will be performed on it and the initial Cartesian coordinate grid is called the physical domain.

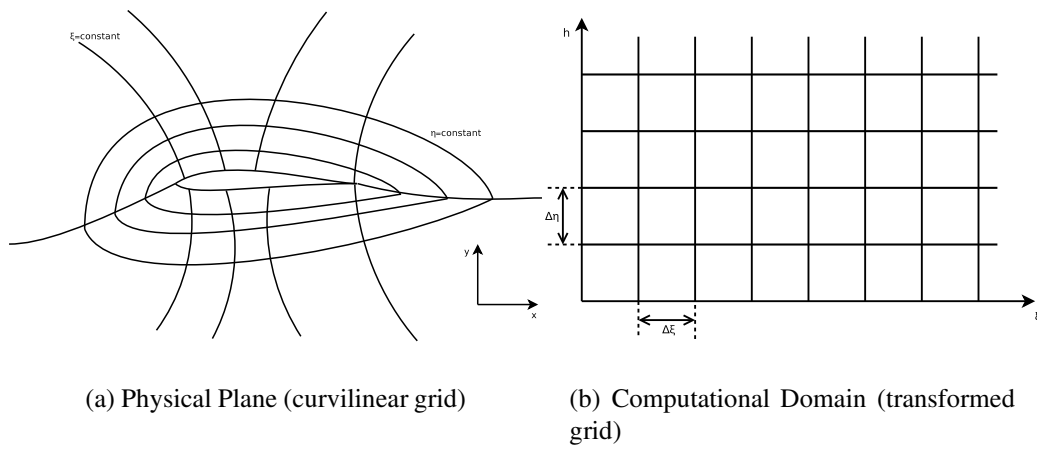


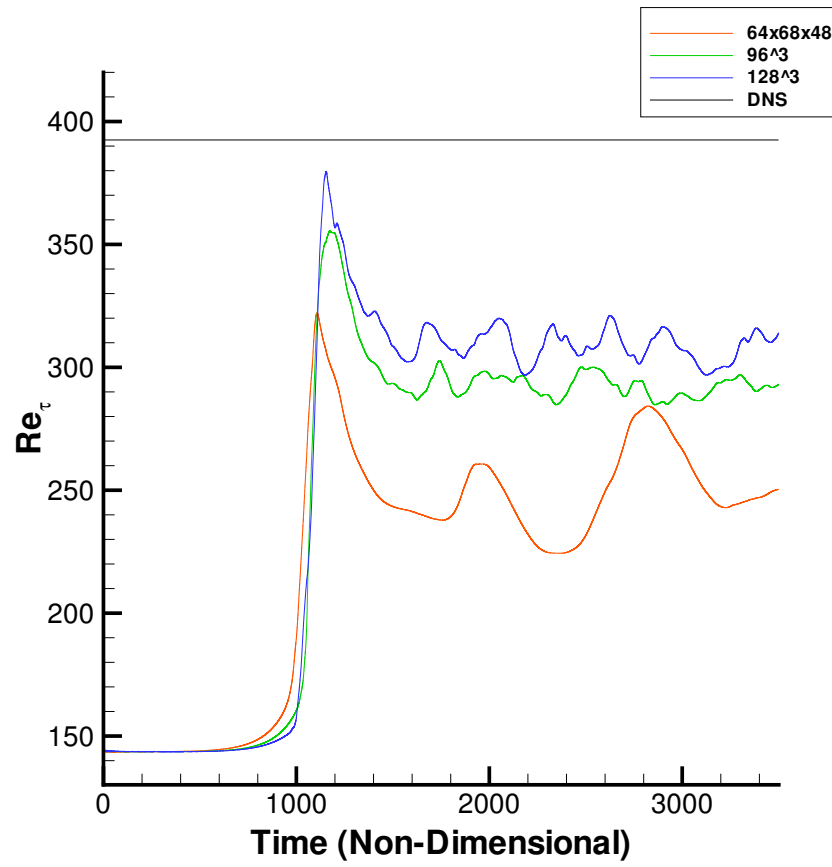
FIGURE B.1: Grid transformation illustrated

C

Appendix C

C.1 No LMNT

C.1.1 Grid Convergence per Limiter

MC LimiterFIGURE C.1: Friction Re obtained on different grids using MC limiter

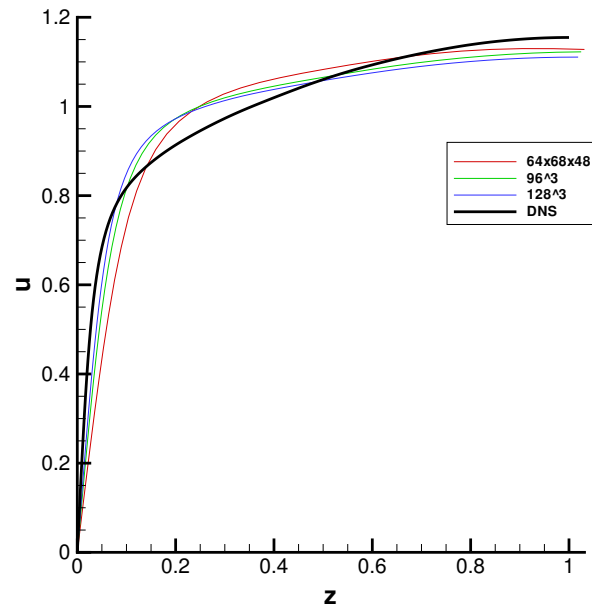
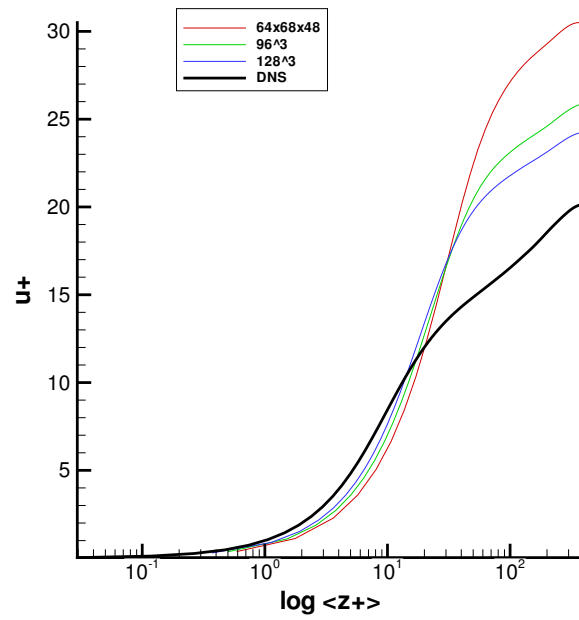
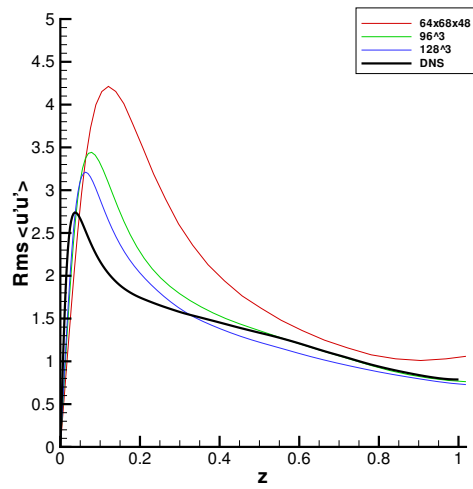
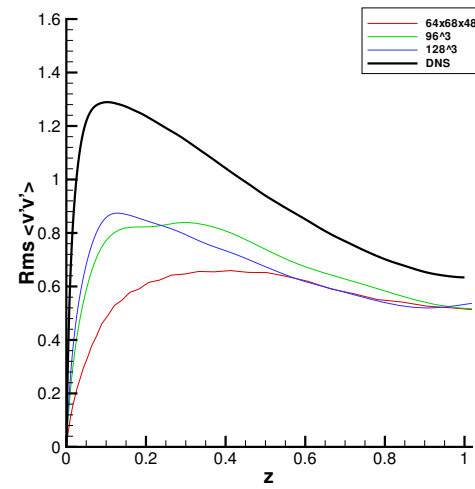
(a) u vs. z (b) u^+ vs. $\log \langle z \rangle$

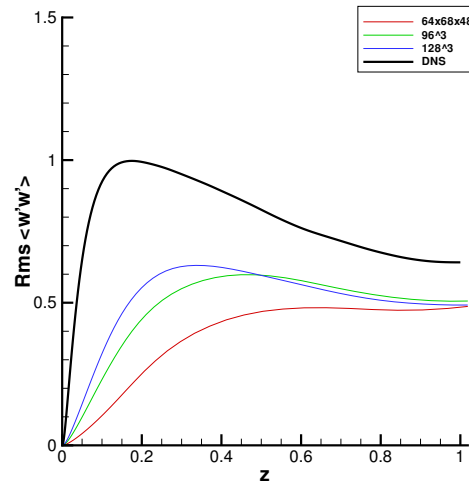
FIGURE C.2: Streamwise velocity profiles obtained on different grids using MC limiter



(a) u



(b) v



(c) w

FIGURE C.3: RMS of velocity components for MC limiter

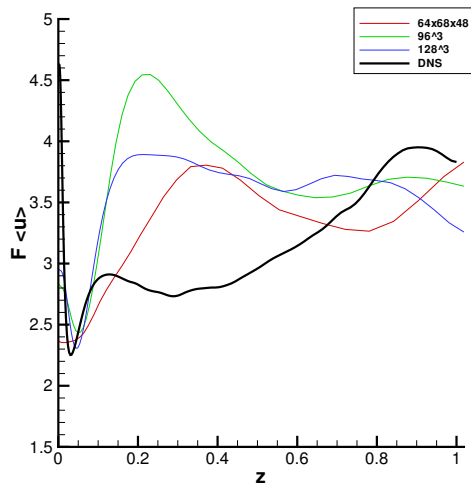
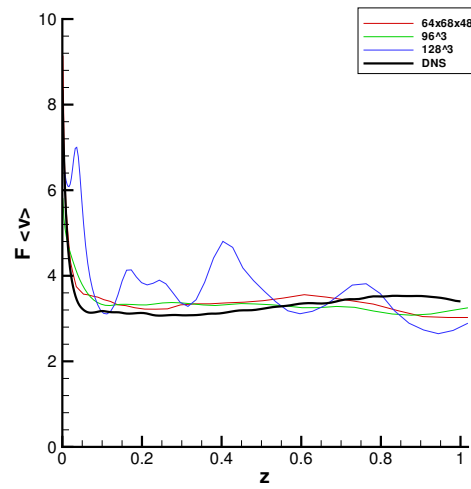
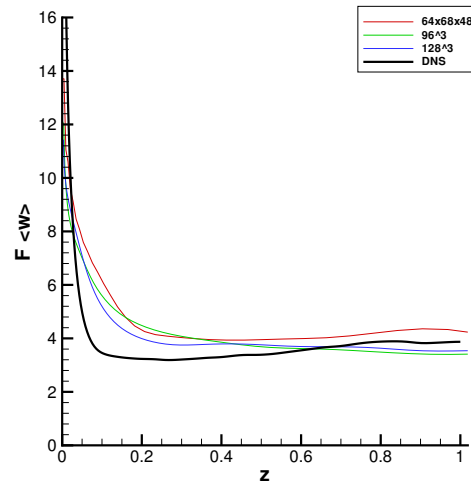
(a) u (b) v (c) w

FIGURE C.4: Flatness of velocity components for MC limiter

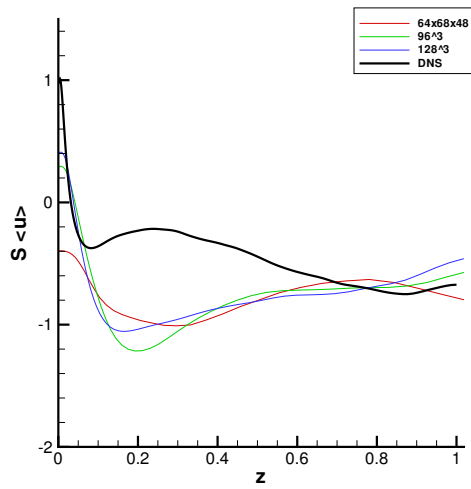
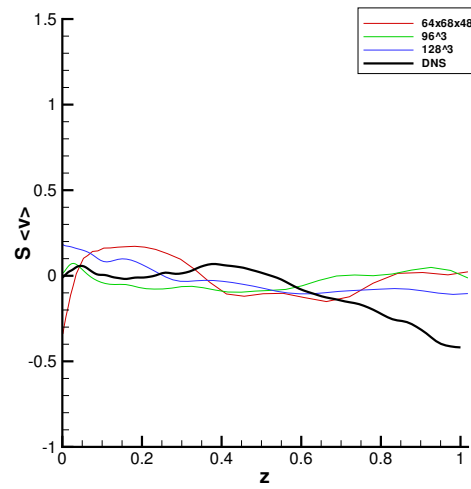
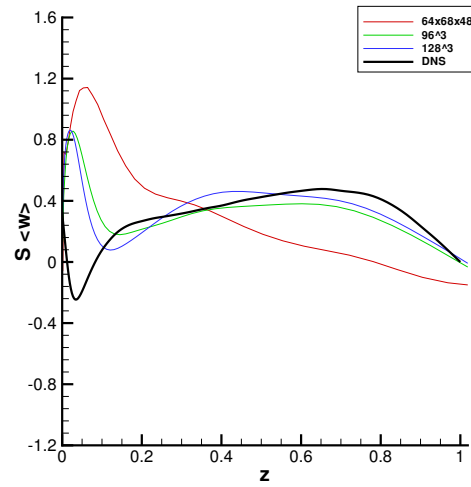
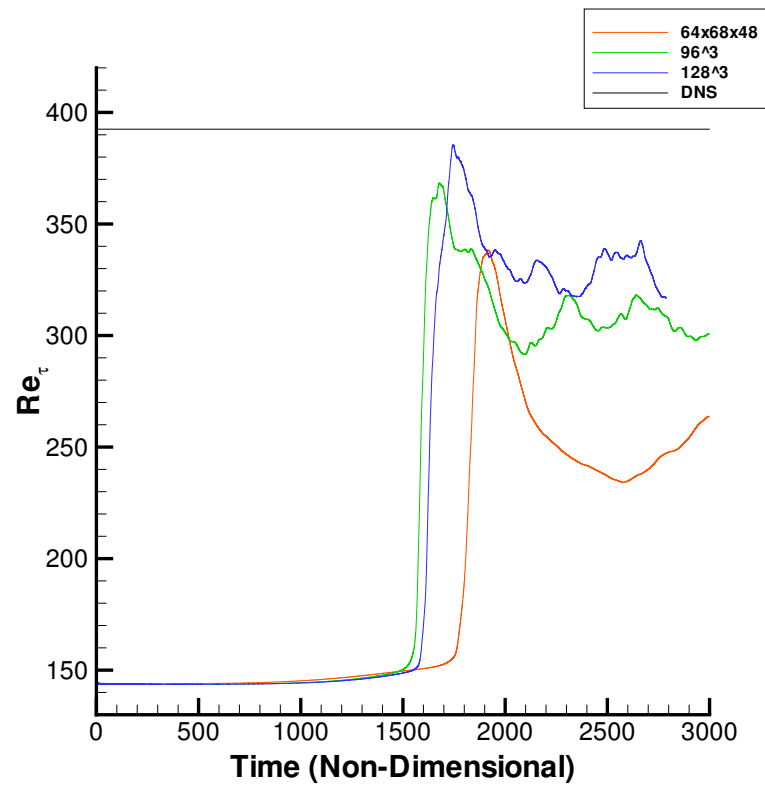
(a) u (b) v (c) w

FIGURE C.5: Skewness of velocity components for MC limiter

M5 LimiterFIGURE C.6: Friction Re obtained on different grids using M5 limiter

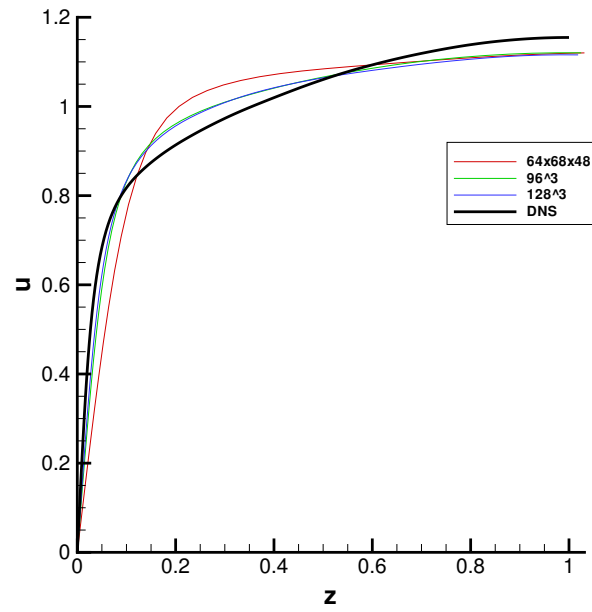
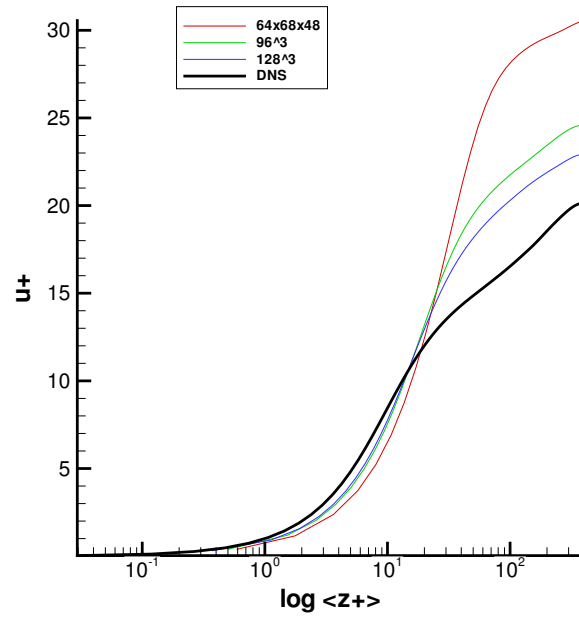
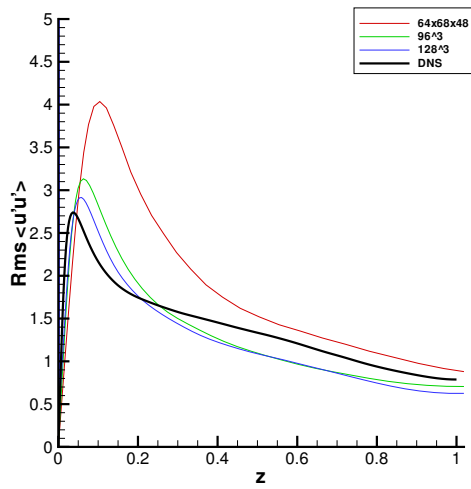
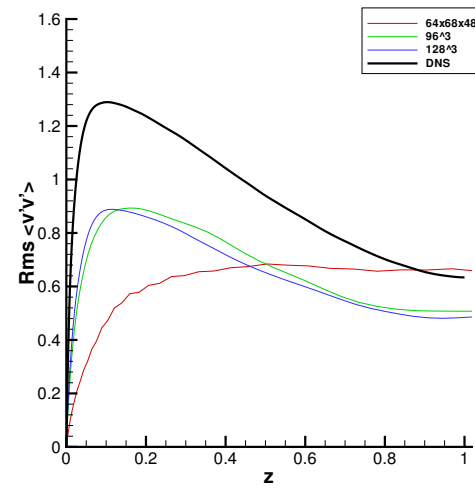
(a) u vs. z (b) u^+ vs. $\log \langle z \rangle$

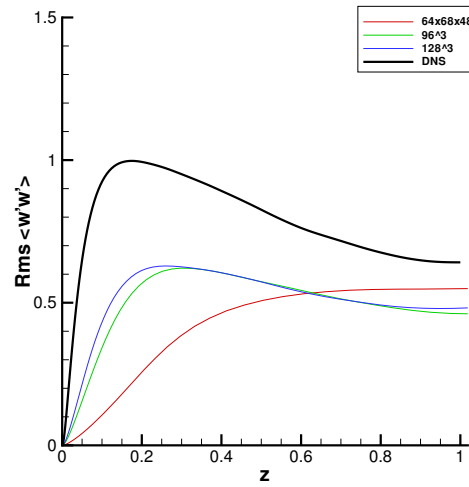
FIGURE C.7: Streamwise velocity profiles obtained on different grids using M5 limiter



(a) u



(b) v



(c) w

FIGURE C.8: RMS of velocity components for M5 limiter

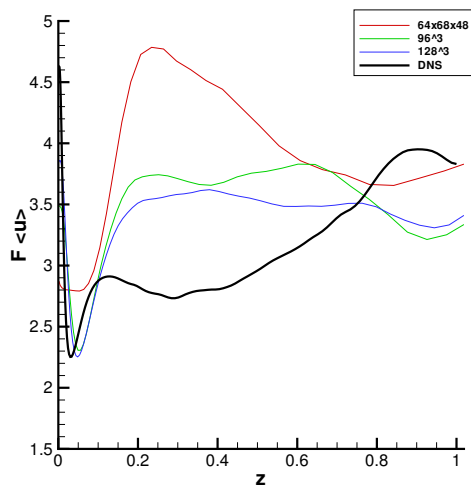
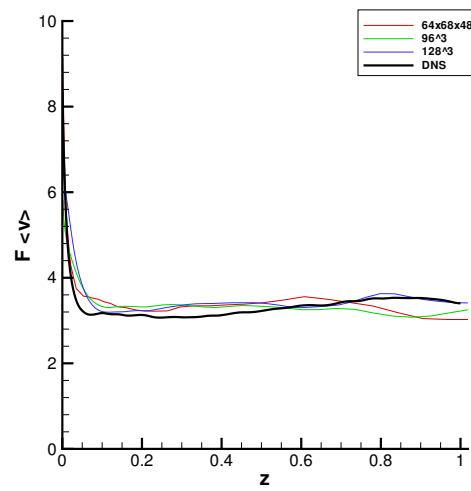
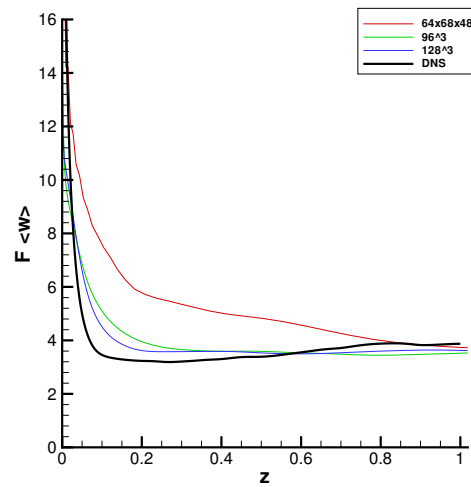
(a) u (b) v (c) w

FIGURE C.9: Flatness of velocity components for M5 limiter

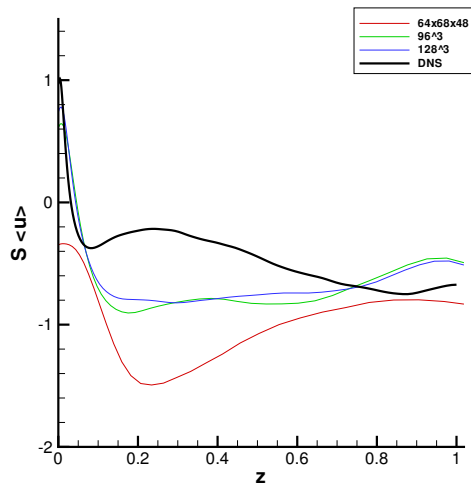
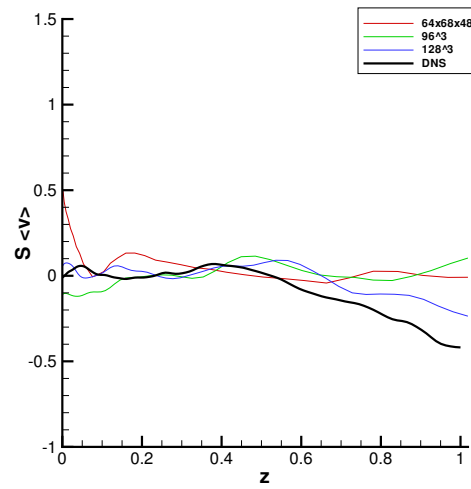
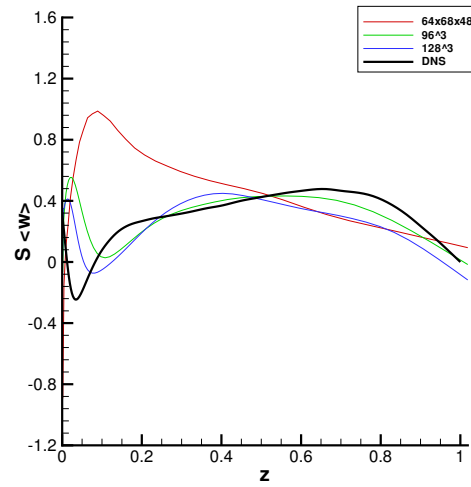
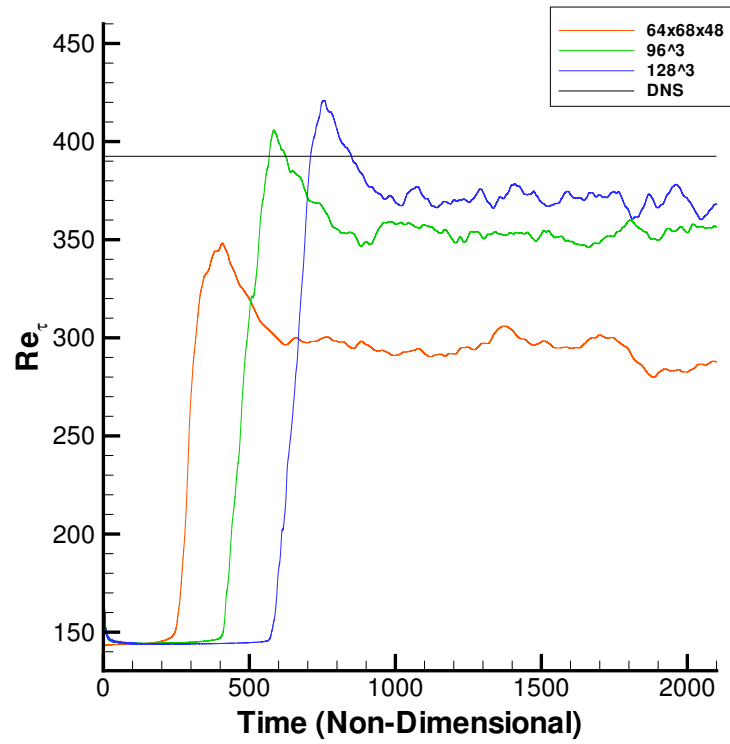
(a) u (b) v (c) w

FIGURE C.10: Skewness of velocity components for M5 limiter

WN9 LimiterFIGURE C.11: Friction Re obtained on different grids using WN9 limiter

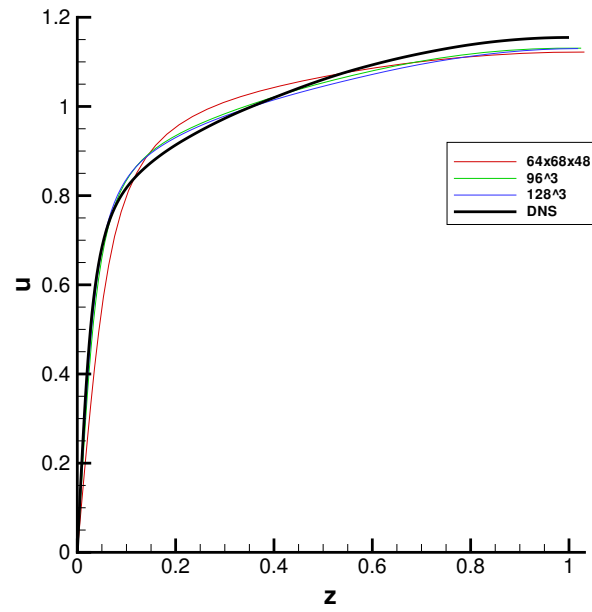
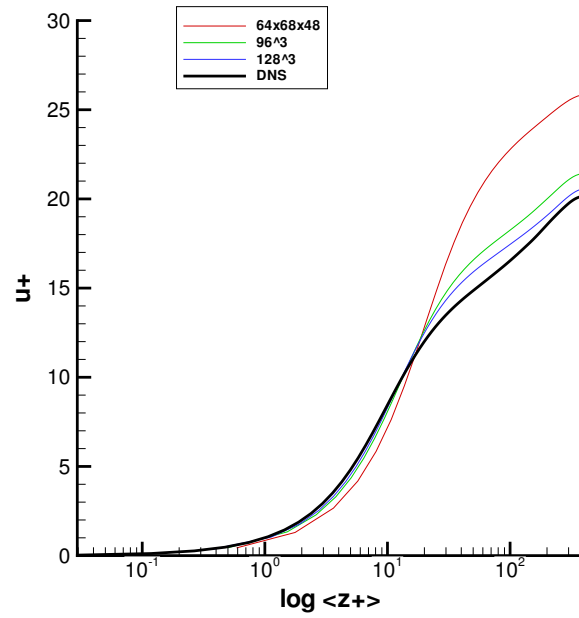
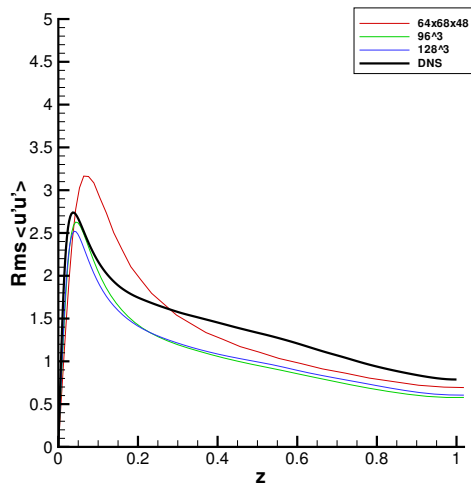
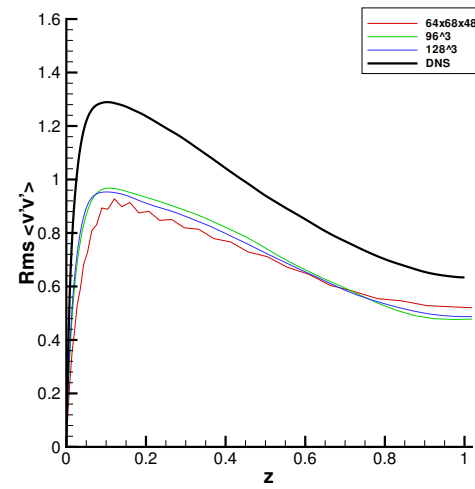
(a) u vs. z (b) u^+ vs. $\log \langle z \rangle$

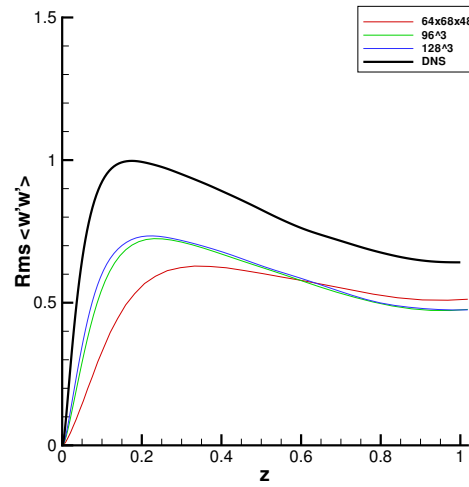
FIGURE C.12: Streamwise velocity profiles obtained on different grids using WN9 limiter



(a) u



(b) v



(c) w

FIGURE C.13: RMS of velocity components for WN9 limiter

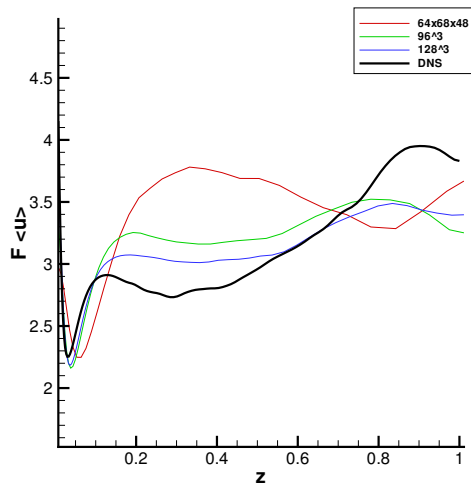
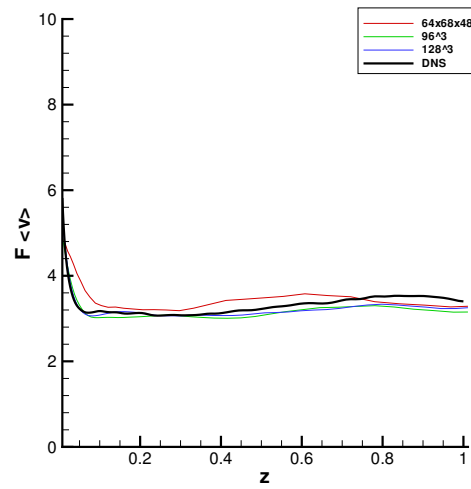
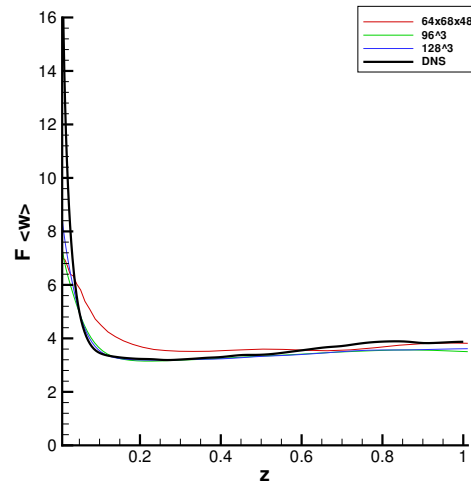
(a) u (b) v (c) w

FIGURE C.14: Flatness of velocity components for WN9 limiter

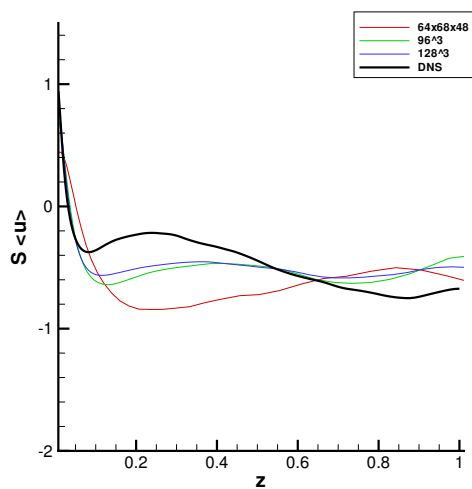
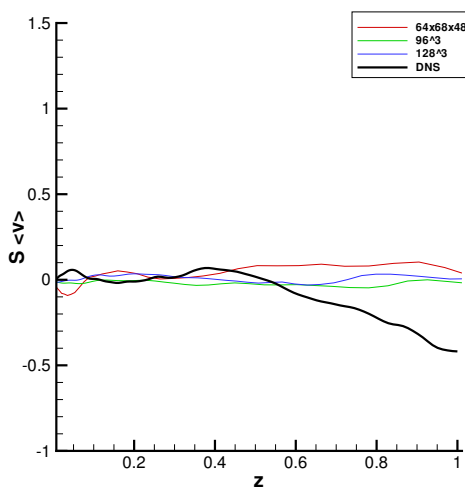
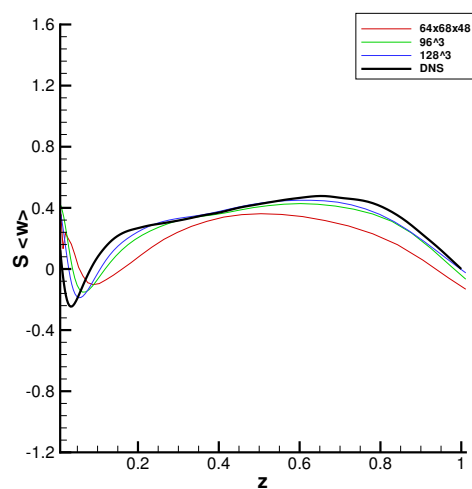
(a) u (b) v (c) w

FIGURE C.15: Skewness of velocity components for WN9 limiter

C.1.2 Limiter Comparison

Hickel's Grid

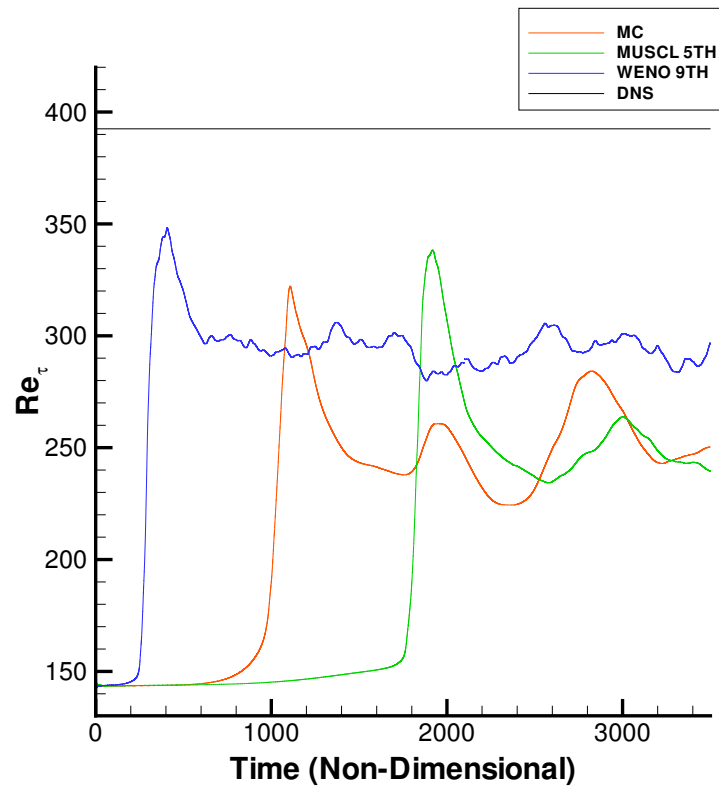


FIGURE C.16: Friction Re obtained on Hickel's grid for different limiters

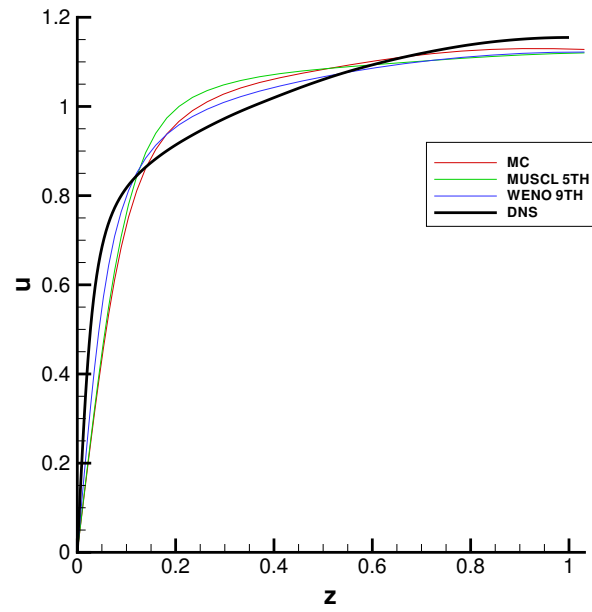
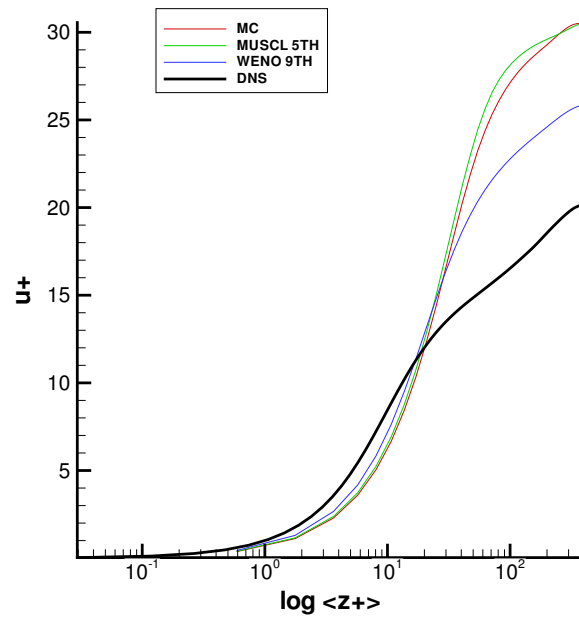
(a) u vs. z (b) u^+ vs. $\log \langle z^+ \rangle$

FIGURE C.17: Streamwise velocity profiles obtained on Hickel's grid for different limiters

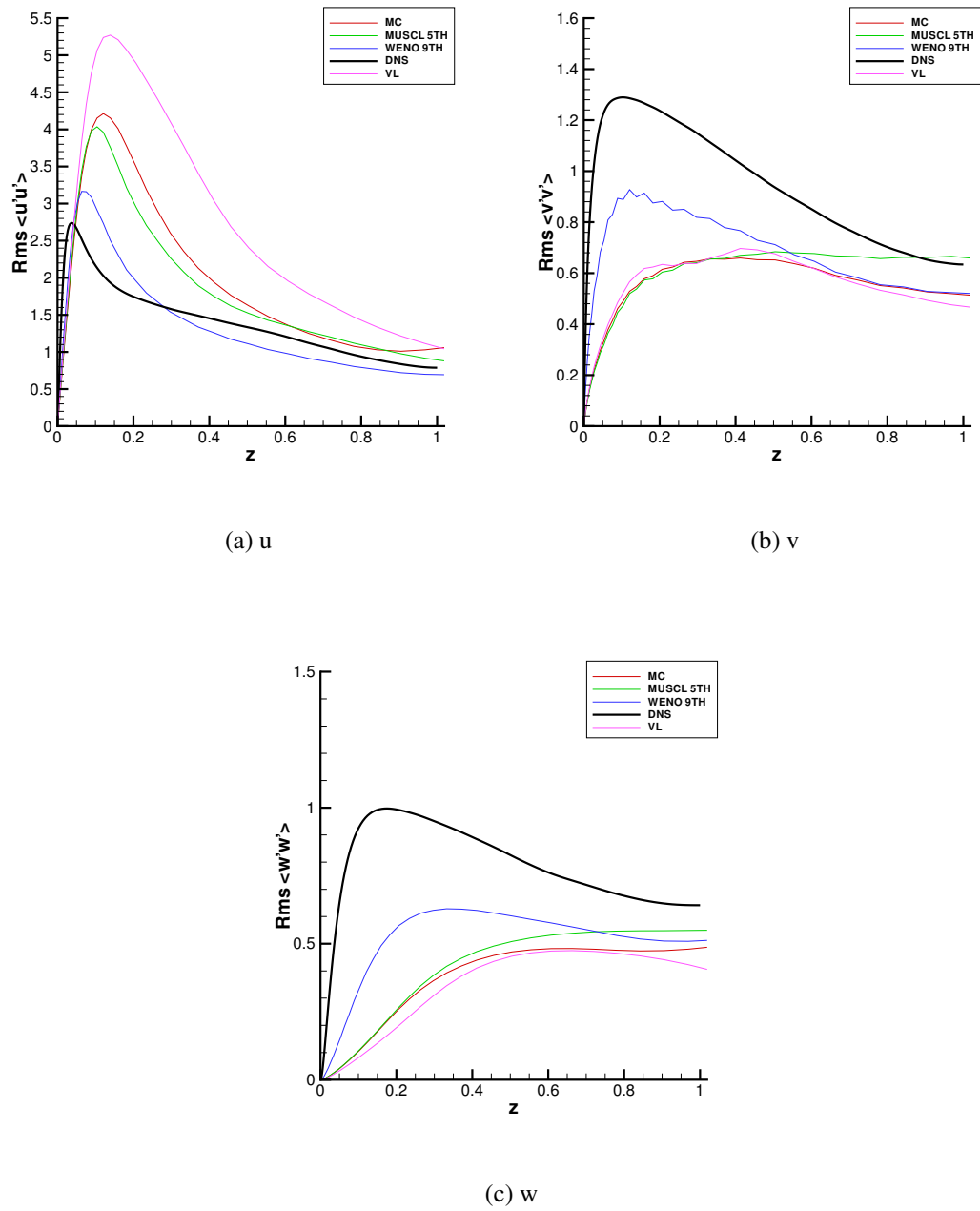
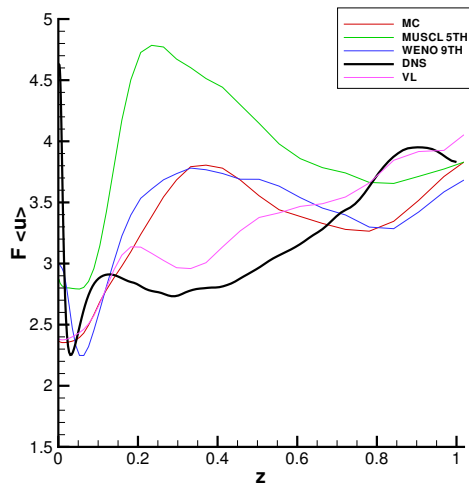
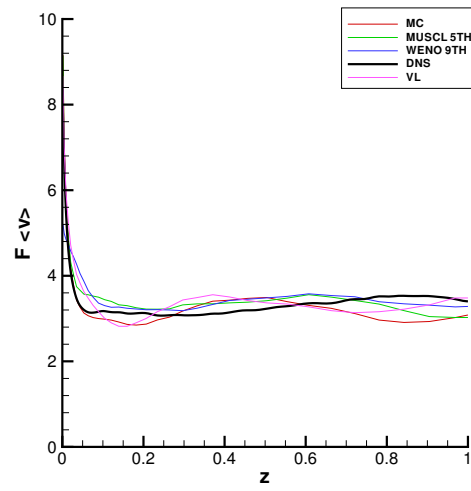


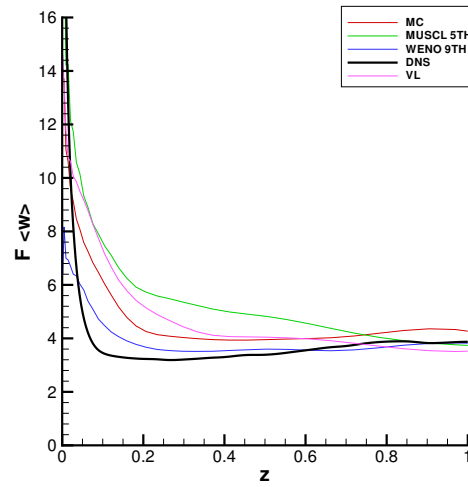
FIGURE C.18: RMS of velocity components on Hickel's grid for different limiters



(a) u



(b) v



(c) w

FIGURE C.19: Flatness of velocity profiles on Hickel's grid for different limiters

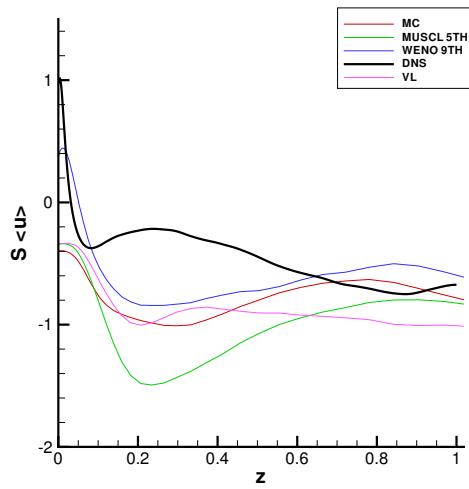
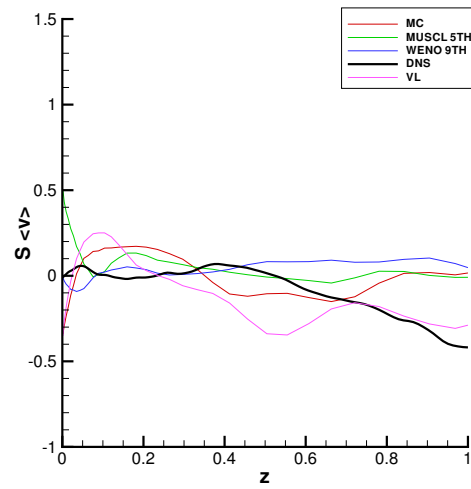
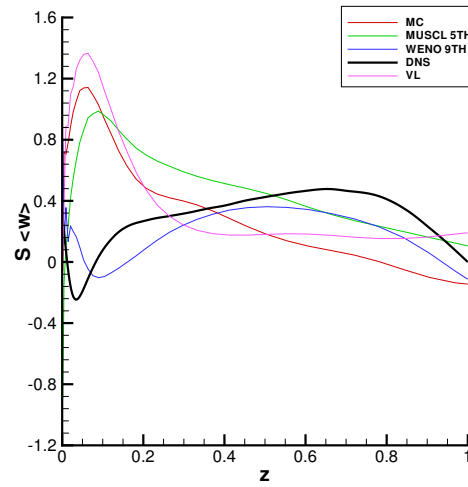
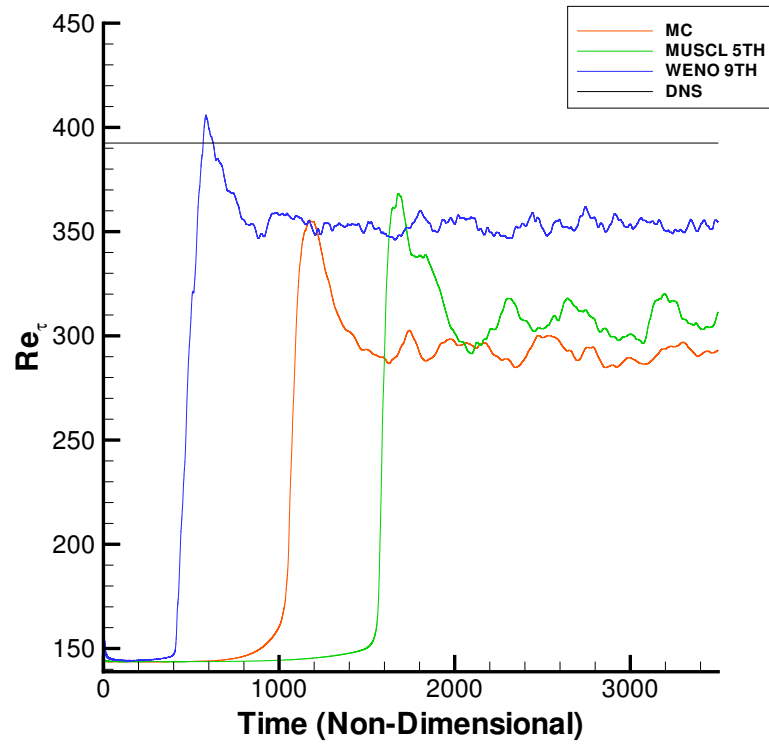
(a) u (b) v (c) w

FIGURE C.20: Skewness of velocity profiles on Hickel's grid for different limiters

96³ GridFIGURE C.21: Friction Re obtained on 96 grid for different limiters

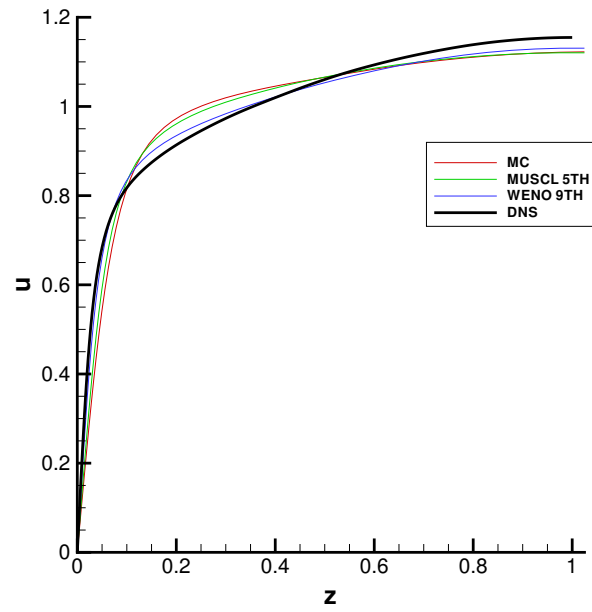
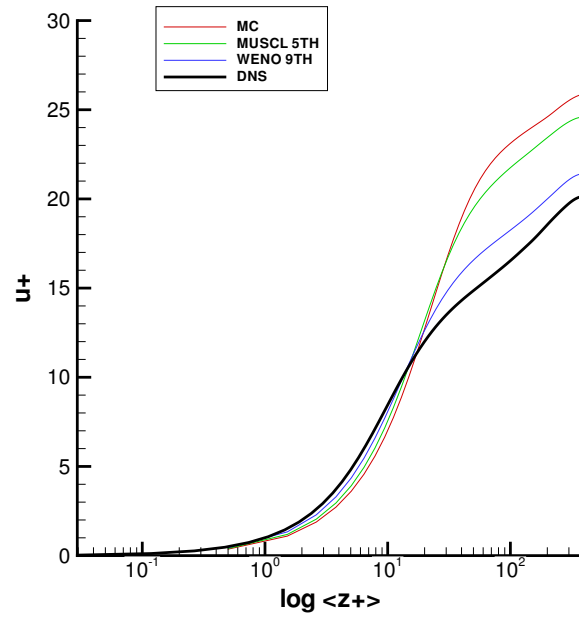
(a) u vs. z (b) u^+ vs. $\log \langle z \rangle$

FIGURE C.22: Streamwise velocity profiles obtained on 96 grid for different limiters

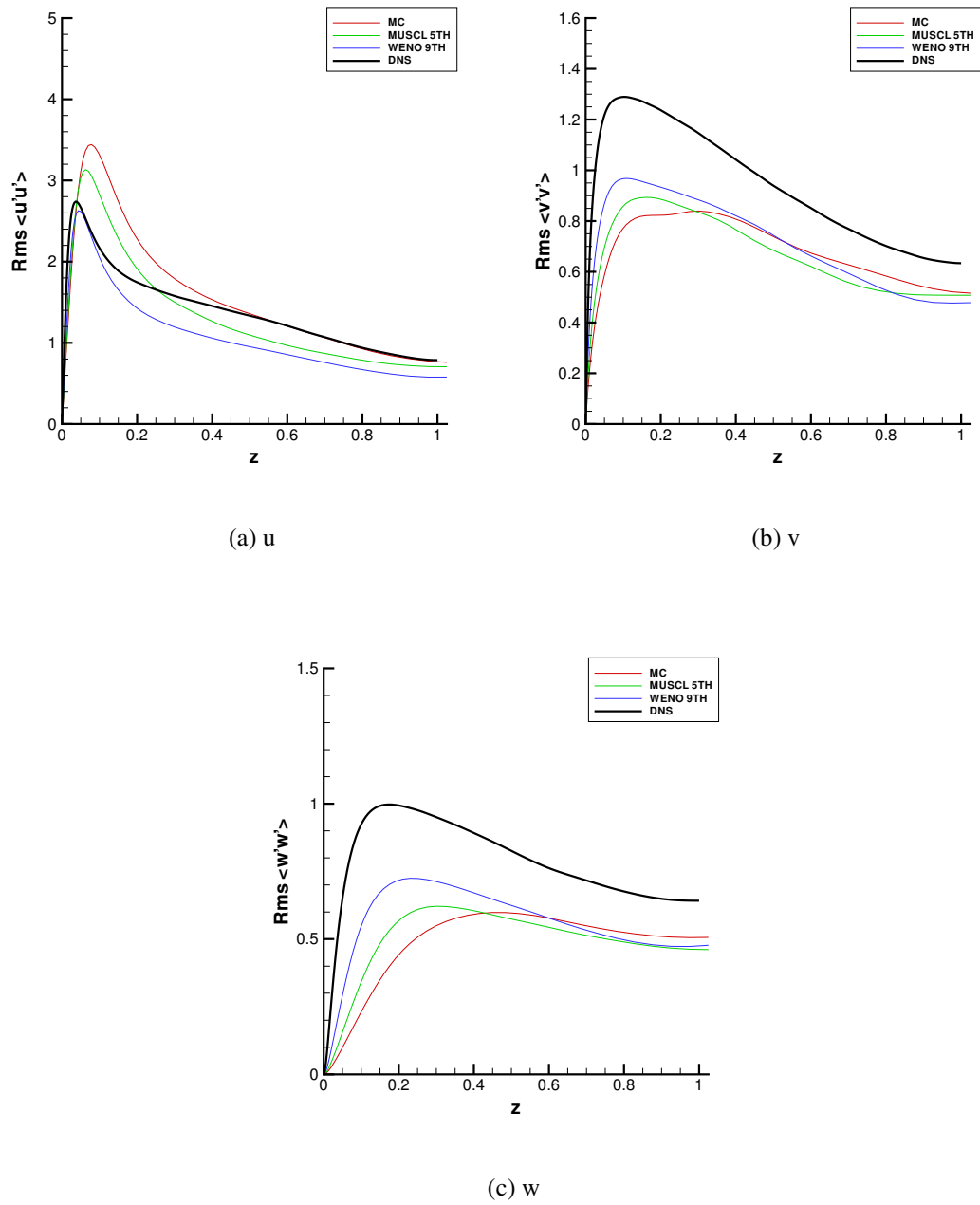


FIGURE C.23: RMS of velocity components on 96 grid for different limiters

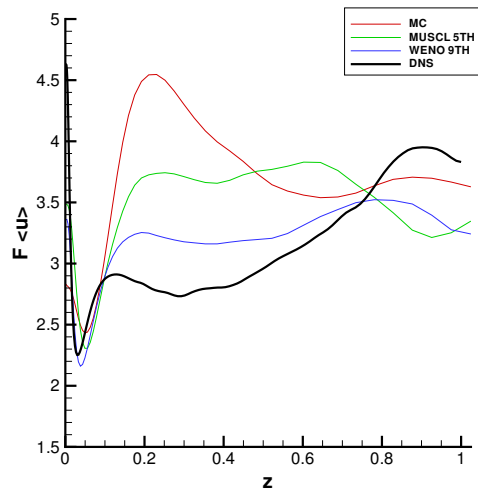
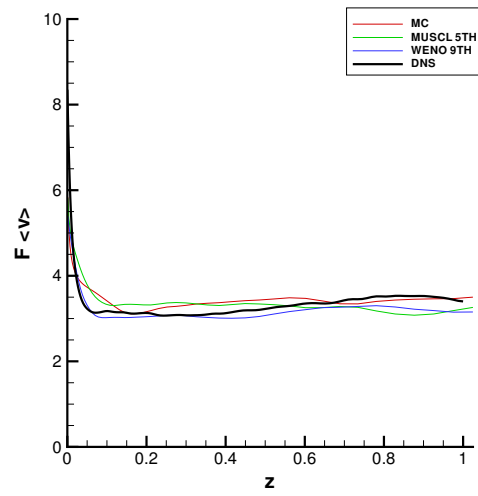
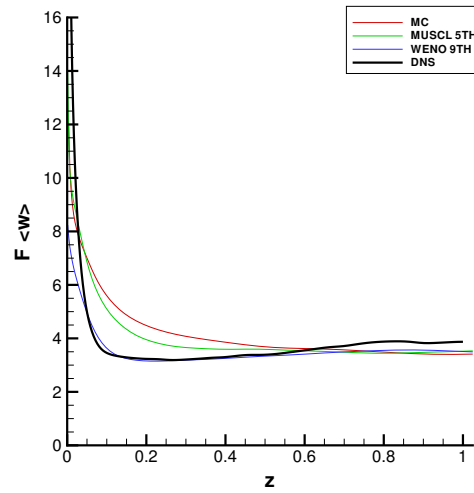
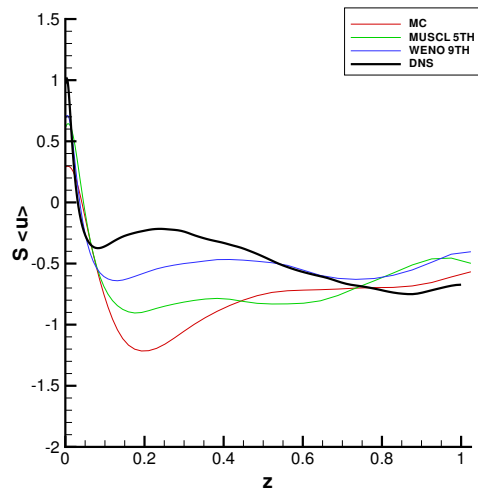
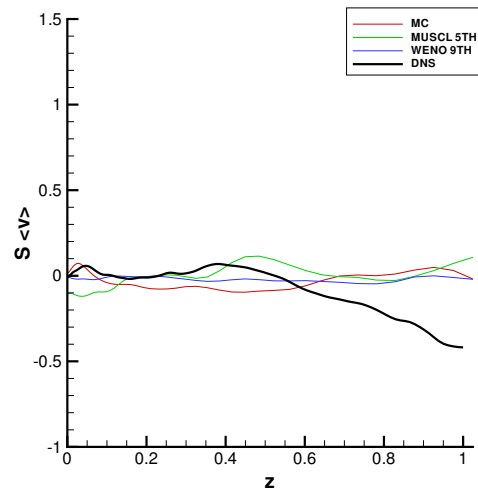
(a) u (b) v (c) w

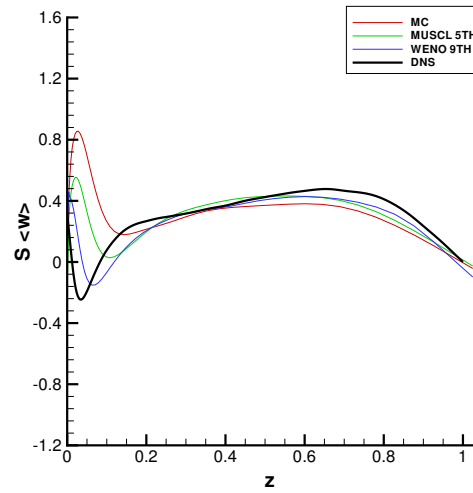
FIGURE C.24: Flatness of velocity profiles on 96 grid for different limiters



(a) u

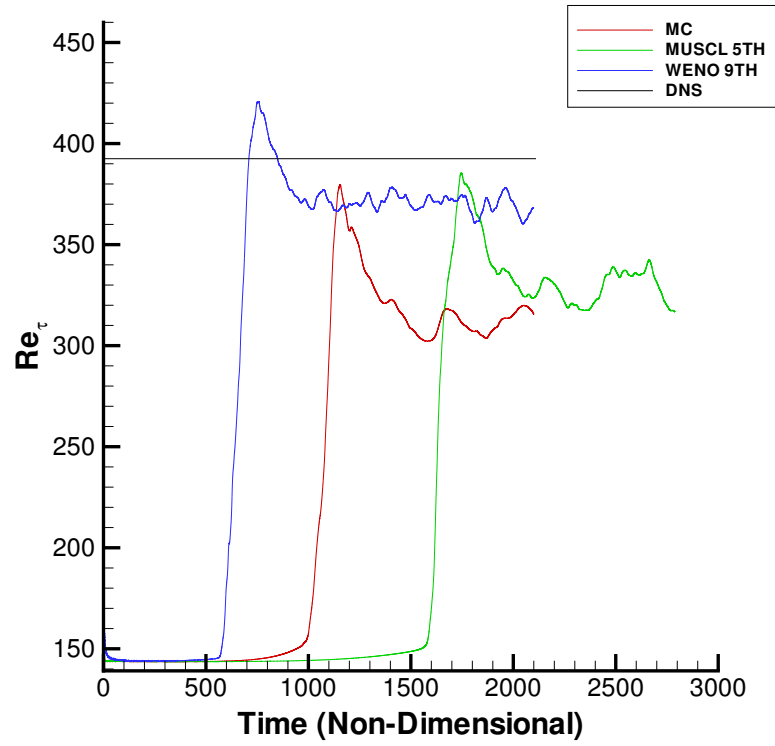


(b) v



(c) w

FIGURE C.25: Skewness of velocity profiles on 96 grid for different limiters

128^3 GridFIGURE C.26: Friction Re obtained on 128 grid for different limiters

C.2 With LMNT

C.2.1 Grid Convergence per Limiter

MC Limiter

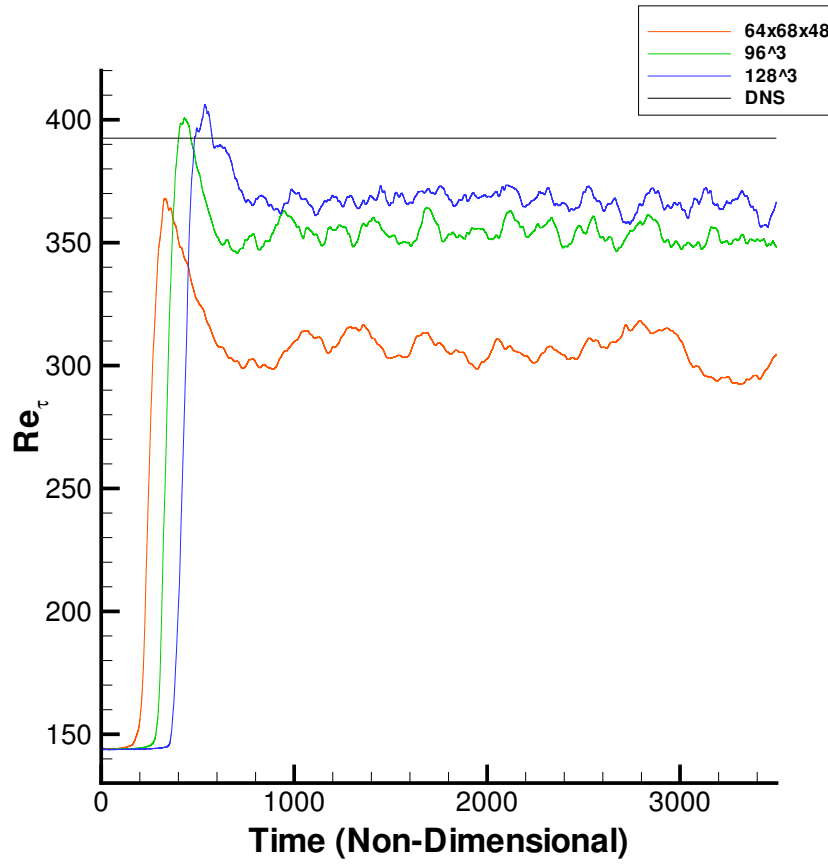
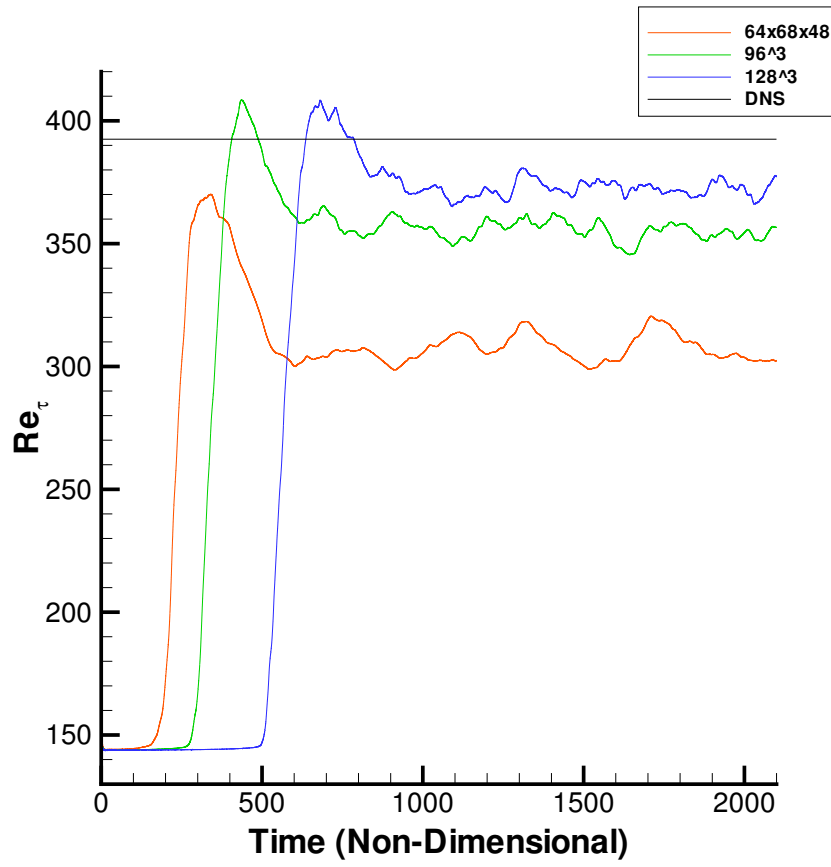
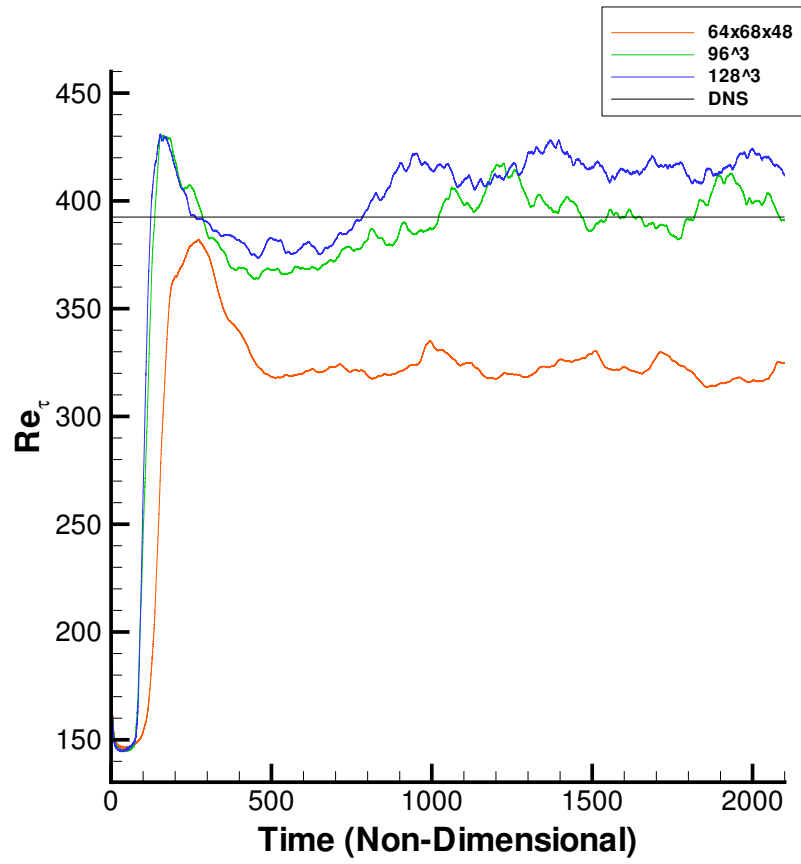


FIGURE C.27: Friction Re obtained on different grids using MC limiter with LMNT

M5 LimiterFIGURE C.28: Friction Re obtained on different grids using M5 limiter with LMNT

WN9 LimiterFIGURE C.29: Friction Re obtained on different grids using WN9 limiter with LMNT

C.2.2 Limiter Comparison

Hickel's Grid

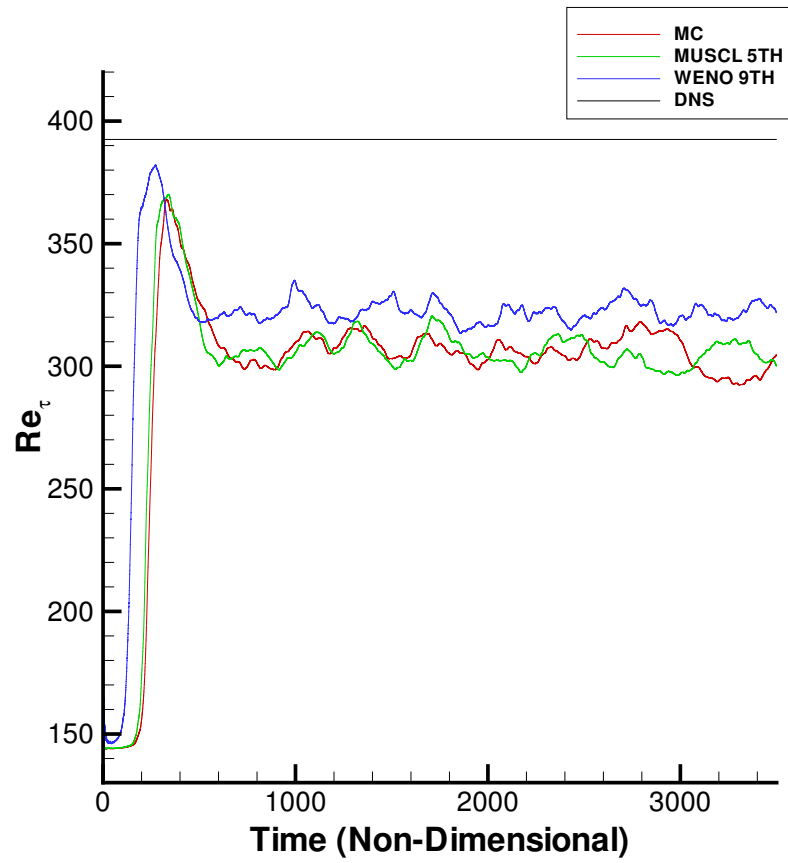
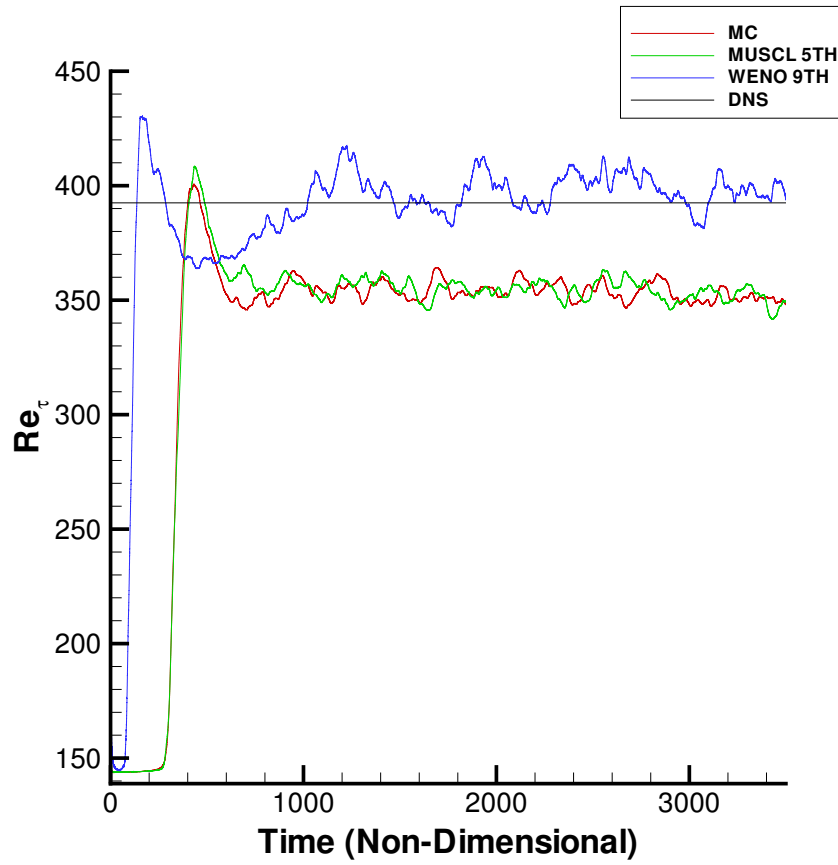


FIGURE C.30: Friction Re obtained on Hickel's grid for different limiters with LMNT

96³ GridFIGURE C.31: Friction Re obtained on 96 grid for different limiters

128³ Grid

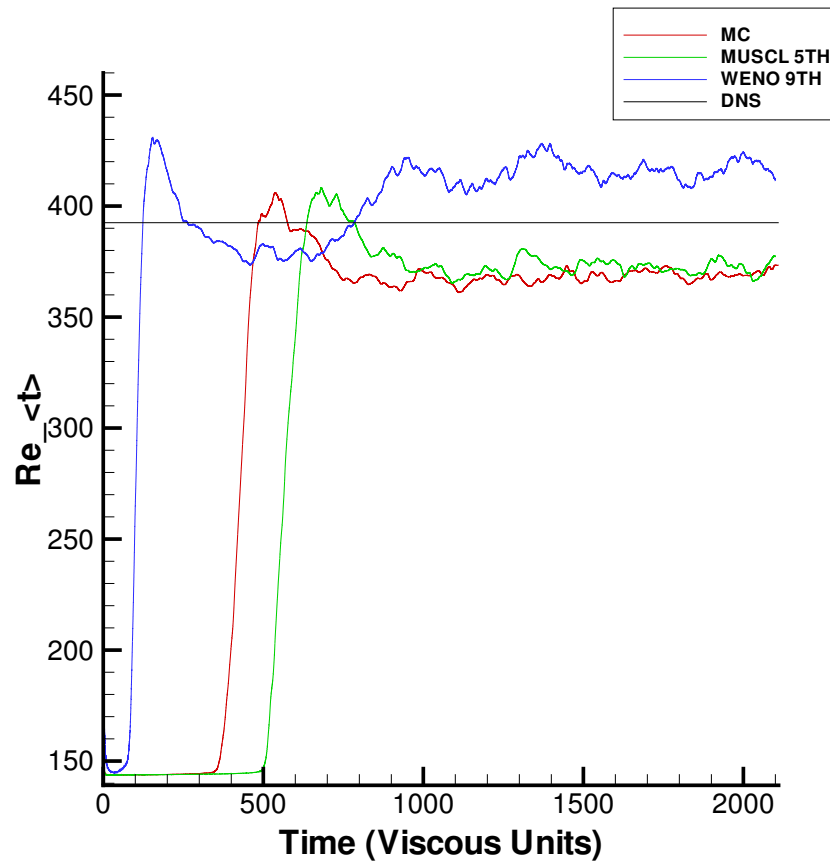


FIGURE C.32: Friction Re obtained on 128 grid for different limiters

D

Appendix D

D.1 Application to CNS3D

D.1.1 Input Reynolds Number

As mentioned in Section 5.3.1, the Reynold's number based on the mean velocity is used for computations. In the following CNS3D variable representation of this section, the following are required to be kept in mind so that the sections are linked:

<i>Theory</i>		<i>CNS3D</i>
Re_m	$\rightarrow$	Re_∞
U_m	$=$	u_∞
δ	$=$	l_∞, l_c

It is important to note that variables denoted with 'c' are used to non-dimensionalize. So now all that is required is to compute the Reynold's number for CNS3D to run successfully. This is accomplished by doing the following:

The theoretical Reynold's number is given as:

$$Re_m = \frac{U_m L}{\nu}$$

where $L = 2\delta$ and therefore:

$$\begin{aligned} Re_m &= \frac{U_m 2\delta}{\nu_\infty} = \frac{u_\infty 2l_c}{\nu_\infty} = 2 \frac{u_\infty l_\infty}{\nu_\infty} \Rightarrow \\ Re_m &= 2Re_\infty \Rightarrow Re_\infty = \frac{Re_m}{2} \end{aligned} \quad (D.1)$$

D.1.2 Non-dimensionalization

Notice that:

$$u_\infty = s_\infty M_\infty$$

and

$$u_c = s_\infty \sqrt{\frac{1 + 0.5\gamma(\gamma - 1) M_\infty^2}{\gamma(\gamma - 1)}}$$

For viscosity:

$$\begin{aligned} Re_\infty &= \frac{u_\infty l_\infty}{\nu_\infty} = \frac{u_c l_c}{\nu_c} \frac{u_\infty^* l_\infty^*}{\nu_\infty^*} = Re_c \frac{u_\infty^*}{\nu_\infty^*} \Rightarrow \\ \frac{\nu_\infty^*}{Re_c} &= \frac{u_\infty^*}{Re_\infty} \end{aligned}$$

Also:

$$\nu_c = \frac{\nu_\infty}{\nu_\infty^*}$$

An important variable to dimensionalize is time. This can be achieved by the equation shown below:

$$\begin{aligned} \tau &= \tau^* \frac{l_c}{u_c} = \tau^* \frac{u_c l_c \nu_c}{u_c^2 \nu_c} = \tau^* \frac{u_c l_c}{\nu_c} \frac{\nu_c}{u_c^2} = \tau^* \frac{Re_c \nu_c}{u_c^2} \Rightarrow \\ \tau &= \tau^* Re_c \frac{\nu_c}{u_c^2} \end{aligned}$$

D.1.3 Mass Flux Preservation

Mass-Flux Preserving Periodic Boundary Condition

In our case a second order discretization is used and therefore 2 ghost cells are required at the boundaries. Figure 5.2 depicts the procedure of the periodic boundary condition with the mass flux conservation, followed by the corresponding formulation used:

1. Outlet Ghosts:

$$\begin{aligned} \rho u(IE1) &= \rho u(2) \times F \\ \rho u(IE) &= \rho u(3) \times F \end{aligned}$$

2. Inlet Ghosts:

$$U(1) = U(IE2) \times F$$

$$U(0) = U(IE3) \times F$$

In order to obtain BETAF, first the mass flux at the inlet (Q_{real}) and the target mass flux (Q_{target}) are required. These can be computed as follows:

$$Q_{target} = u_{\infty}^* L_y L_z = Q * 2 * 3.141$$

where $(L_y, L_z) = (2\pi, 2)$ in this case.

And

$$Q_{real} = \sum_{K=2}^{KE2} \left\{ \sum_{J=2}^{JE2} [U(2, J, K) \times area(2, J, K)] \right\}$$

where

$$DY(2, J, K) = \frac{[y(2, J+1, K) - y(2, J, K)] + [y(2, J+1, K+1) - y(2, J, K+1)]}{2}$$

$$DZ(2, J, K) = \frac{[z(2, J, K+1) - z(2, J, K)] + [z(2, J+1, K+1) - z(2, J+1, K)]}{2}$$

$$area(2, J, K) = DY(2, J, K) \times DZ(2, J, K)$$

,so

$$F = \frac{Q_{target}}{Q_{real}}$$

The variable 'area' is the area of the cell face in the Y-Z plane of the cell with velocity U. An illustration of this can be seen below in Figure D.1.

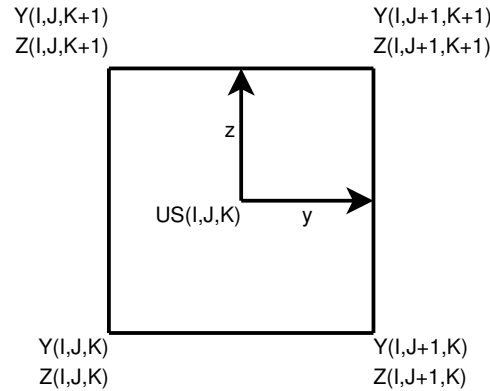


FIGURE D.1: Cell-Point Correspondence

The reason index I is selected to be equal to 2 in the mass flux calculation is cause I=2 refers to the first cell at the inlet. The computational domain ghost relationship can be visualized using the following 1-Dimensional illustration in Figure D.2.

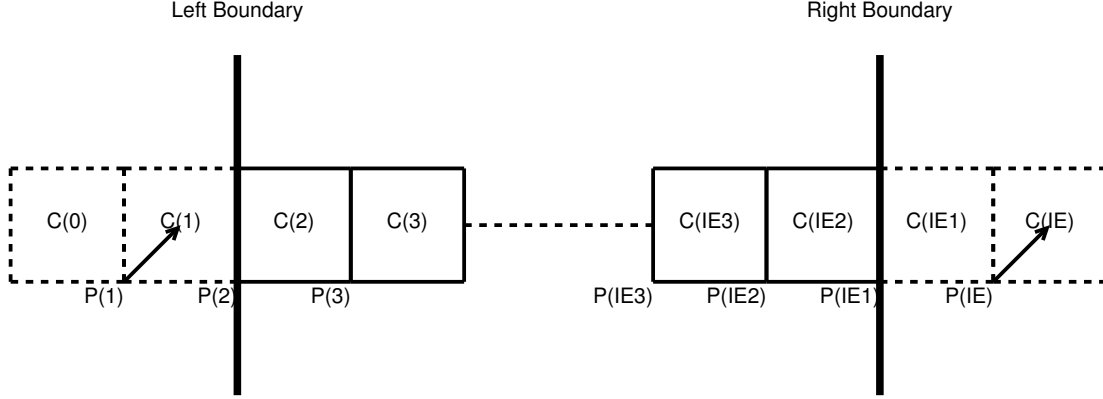


FIGURE D.2: 1-Dimensional boundary indexing of points and cells

D.2 Additional Information

D.2.1 DNS - CNS3D comparisons

It is not unusual for different codes to use different nondimensionalizing variables. This is the case with the DNS data available from [35] and the CNS3D code. In the comparisons above this problem was stumbled upon when trying to compare the mean streamwise velocity profile divided by the bulk velocity and to obtain the streamwise velocity slope. The former and latter problems were resolved by using Equation (D.2) and D.3:

$$\frac{u}{u_\tau} = \frac{u}{u_\infty} \frac{u_\infty}{u_\tau} = \frac{u}{u_\infty} \frac{\frac{u_\infty l_\infty}{\nu_\infty}}{\frac{u_\tau l_\infty}{\nu_\infty}} = \frac{u}{u_\infty} \frac{Re_\infty}{Re_\tau} \Rightarrow$$

$$\frac{u}{u_\infty} = \frac{Re_\tau}{Re_\infty} \frac{u}{u_\tau} \quad (D.2)$$

and

$$\frac{u}{u_\infty} = \frac{u}{U_c} \frac{U_c}{u_\infty} = \frac{u}{U_c} \frac{1}{u_\infty^*} \Rightarrow$$

$$\frac{u}{U_c} = u_\infty^* \frac{u}{u_\infty} \quad (\text{D.3})$$

In the case of u^+ there was no problem since the reference velocity used to nondimensionalize velocity is canceled out. This is shown below:

$$u^+ = \frac{\langle U^* \rangle}{u_\tau^*} = \frac{\left\langle \frac{U}{U_{ref}} \right\rangle}{\frac{u_\tau}{U_{ref}}} = \frac{\frac{\langle U \rangle}{U_{ref}}}{\frac{u_\tau}{U_{ref}}} = \frac{\langle U \rangle}{u_\tau}$$