NUMERICAL INVESTIGATION OF
SUPersonic Turbulent
Boundary Layers

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presented by
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"Monseigneur, la difficulté de réussir ne fait qu’ajouter à la nécessité d’entreprendre."

*Figaro au Comte dans Le Barbier de Séville, acte premier, scène VI*  
(*Pierre Augustin Caron de Beaumarchais*)

"L’Homme se découvre quand il se mesure avec l’obstacle."

*Terre des hommes* (*Antoine de Saint-Exupéry*)
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<td>$b_{ij}$</td>
<td>Reynolds stress anisotropy tensor</td>
<td>(8.11)</td>
</tr>
<tr>
<td>$c$</td>
<td>speed of sound</td>
<td>(3.20)</td>
</tr>
<tr>
<td>$c_p$</td>
<td>specific heat at constant pressure</td>
<td></td>
</tr>
<tr>
<td>$c_v$</td>
<td>specific heat at constant volume</td>
<td></td>
</tr>
<tr>
<td>$C_f$</td>
<td>skin-friction coefficient</td>
<td>(6.3)</td>
</tr>
<tr>
<td>$E$</td>
<td>total energy</td>
<td>(2.3)</td>
</tr>
<tr>
<td>$F$</td>
<td>flux vector in $x$-direction</td>
<td>(2.4)</td>
</tr>
<tr>
<td>$G$</td>
<td>flux vector in $y$-direction</td>
<td>(2.5)</td>
</tr>
<tr>
<td>$h$</td>
<td>grid spacing in the basic interval for the</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$z$-mapping</td>
<td></td>
</tr>
<tr>
<td>$H$</td>
<td>flux vector in $z$-direction</td>
<td>(2.6)</td>
</tr>
<tr>
<td>$H_{12}$</td>
<td>shape factor</td>
<td></td>
</tr>
<tr>
<td>$i$</td>
<td>imaginary unit</td>
<td></td>
</tr>
<tr>
<td>$J$</td>
<td>Jacobian matrix</td>
<td>(2.35)</td>
</tr>
<tr>
<td>$k_x, k_y$</td>
<td>wave number</td>
<td></td>
</tr>
<tr>
<td>$K$</td>
<td>turbulent kinetic energy per unit mass</td>
<td>(6.43)</td>
</tr>
<tr>
<td>$l_x, l_y, l_z$</td>
<td>dimensions of the computational domain</td>
<td></td>
</tr>
<tr>
<td>$\mathcal{L}$</td>
<td>integral length</td>
<td>(6.9)</td>
</tr>
<tr>
<td>$m$</td>
<td>metric coefficient for the $z$-mapping</td>
<td>(3.9, 3.10)</td>
</tr>
<tr>
<td>$M$</td>
<td>Mach number</td>
<td></td>
</tr>
<tr>
<td>$M'$</td>
<td>fluctuating Mach number</td>
<td>(6.11)</td>
</tr>
<tr>
<td>$M_c$</td>
<td>convective Mach number</td>
<td>(8.9)</td>
</tr>
<tr>
<td>$M_g$</td>
<td>gradient Mach number</td>
<td>(8.4)</td>
</tr>
<tr>
<td>$M_{rel}$</td>
<td>relative Mach number</td>
<td>(7.1)</td>
</tr>
<tr>
<td>$M_t$</td>
<td>turbulence Mach number</td>
<td>(6.10)</td>
</tr>
<tr>
<td>$M_{tr}$</td>
<td>transverse Mach number</td>
<td>(8.10)</td>
</tr>
<tr>
<td>$n_s$</td>
<td>number of samples for the turbulence statistics</td>
<td></td>
</tr>
<tr>
<td>$N$</td>
<td>number of gridpoints in a certain direction</td>
<td></td>
</tr>
<tr>
<td>$p$</td>
<td>pressure</td>
<td></td>
</tr>
<tr>
<td>$\mathcal{P}$</td>
<td>turbulence production per unit mass</td>
<td>(6.45)</td>
</tr>
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### Nomenclature

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<th>Description</th>
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<tr>
<td>( Pr )</td>
<td>Prandtl number</td>
</tr>
<tr>
<td>( Pr_t )</td>
<td>turbulent Prandtl number (6.24)</td>
</tr>
<tr>
<td>( q )</td>
<td>heat flux vector (2.14)</td>
</tr>
<tr>
<td>( Q )</td>
<td>vector of characteristic variables (2.16)</td>
</tr>
<tr>
<td>( R )</td>
<td>gas constant</td>
</tr>
<tr>
<td>( R_{u'' T''} )</td>
<td>coefficient of correlation between ( u'' ) and ( T'' ) (6.23)</td>
</tr>
<tr>
<td>( Re )</td>
<td>computational Reynolds number (2.9)</td>
</tr>
<tr>
<td>( Re_t )</td>
<td>turbulence Reynolds number</td>
</tr>
<tr>
<td>( Re_{\delta_1} )</td>
<td>Reynolds number based on ( \delta_1 )</td>
</tr>
<tr>
<td>( Re_{\delta_2} )</td>
<td>Reynolds number based on ( \delta_2 )</td>
</tr>
<tr>
<td>( Re_{\theta} )</td>
<td>Reynolds number based on ( \delta_2 ) and ( \mu_w )</td>
</tr>
<tr>
<td>( Re_{T} )</td>
<td>Reynolds number based on the channel half-width and skin-friction velocity</td>
</tr>
<tr>
<td>( S )</td>
<td>mean shear rate</td>
</tr>
<tr>
<td>( St )</td>
<td>Stanton number (7.2)</td>
</tr>
<tr>
<td>( Su )</td>
<td>Sutherland's constant</td>
</tr>
<tr>
<td>( t )</td>
<td>time</td>
</tr>
<tr>
<td>( t_s )</td>
<td>sampling period</td>
</tr>
<tr>
<td>( T )</td>
<td>static temperature</td>
</tr>
<tr>
<td>( T_0 )</td>
<td>total temperature (6.14)</td>
</tr>
<tr>
<td>( u \equiv u_1 )</td>
<td>streamwise velocity component</td>
</tr>
<tr>
<td>( u_T )</td>
<td>friction velocity (6.5)</td>
</tr>
<tr>
<td>( U )</td>
<td>vector of conservative variables</td>
</tr>
<tr>
<td>( v \equiv u_2 )</td>
<td>spanwise velocity component</td>
</tr>
<tr>
<td>( w \equiv u_3 )</td>
<td>wall-normal velocity component</td>
</tr>
<tr>
<td>( x \equiv x_1 )</td>
<td>“fast” streamwise coordinate related to smaller scale phenomena</td>
</tr>
<tr>
<td>( x_g )</td>
<td>general streamwise coordinate</td>
</tr>
<tr>
<td>( X )</td>
<td>“slow” streamwise coordinate related to larger scale phenomena, streamwise position of the computational domain</td>
</tr>
<tr>
<td>( y \equiv x_2 )</td>
<td>spanwise coordinate</td>
</tr>
<tr>
<td>( z \equiv x_3 )</td>
<td>wall-normal coordinate</td>
</tr>
<tr>
<td>( Z_0, Z_1, Z_c )</td>
<td>forcing terms (2.31, 2.33, 2.48)</td>
</tr>
<tr>
<td>( II, III )</td>
<td>invariants of the Reynolds stress anisotropy tensor (8.12, 8.13)</td>
</tr>
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</table>
Greek symbols

\( \gamma \) \quad \text{ratio of specific heats} (2.11)
\( \delta_c \) \quad \text{compressible thickness} (2.11)
\( \delta_0 \) \quad \text{boundary-layer thickness} (2.10)
\( \delta_1 \) \quad \text{displacement thickness} (2.12)
\( \delta_2 \) \quad \text{momentum thickness} (2.13)
\( \delta_{ij} \) \quad \text{Kronecker’s delta}
\( \Delta_x, \Delta_y, \Delta_z \) \quad \text{grid spacing of the computational domain} (6.49)
\( \epsilon \) \quad \text{turbulent dissipation per unit mass}
\( \eta \) \quad \text{Kolmogorov length scale}
\( \kappa \) \quad \text{von Kármán’s constant}
\( \lambda \) \quad \text{mean free-path / thermal conductivity}
\( \lambda_i \) \quad \text{scalar eigenvalue}
\( \Lambda \) \quad \text{vector of eigenvalues} (A.5)
\( \mu \) \quad \text{dynamic viscosity} (2.8)
\( \nu \) \quad \text{kinematic viscosity}
\( \rho \) \quad \text{density}
\( \tau \) \quad \text{shear stress / time step} (2.7)
\( \tau_{ij} \) \quad \text{viscous stress tensor}
\( (\xi, \eta, \zeta) \) \quad \text{tilted coordinate system}

Other symbols

\( \nabla \) \quad \text{derivation operator}
\( \otimes \) \quad \text{dyadic product}

Subscripts

\( \infty \) \quad \text{free-stream properties}
\( \text{lam} \) \quad \text{laminar}
\( P \) \quad \text{parabolized}
\( S \) \quad \text{solenoidal}
\( t \) \quad \text{turbulent}
\( VD \) \quad \text{transformed according to van Driest}
\( w \) \quad \text{properties at the wall}
### Superscripts

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<tr>
<td>*</td>
<td>dimensional values</td>
</tr>
<tr>
<td>+</td>
<td>wall units (scaled with $u_\tau, \nu_w$)</td>
</tr>
<tr>
<td>*</td>
<td>semi-local scaling</td>
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### Abbreviations

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<tr>
<td>AIM</td>
<td>anisotropy-invariant map</td>
</tr>
<tr>
<td>CFL</td>
<td>Courant - Friedrich - Levy</td>
</tr>
<tr>
<td>CPU</td>
<td>central processing unit</td>
</tr>
<tr>
<td>DNS</td>
<td>direct numerical simulation</td>
</tr>
<tr>
<td>DRAM</td>
<td>dynamic random access memory</td>
</tr>
<tr>
<td>ETDNS</td>
<td>extended temporal direct numerical simulation</td>
</tr>
<tr>
<td>FD</td>
<td>finite difference</td>
</tr>
<tr>
<td>FFT</td>
<td>fast Fourier transform</td>
</tr>
<tr>
<td>FLOPS</td>
<td>floating-point operations per second</td>
</tr>
<tr>
<td>ODE</td>
<td>ordinary differential equation</td>
</tr>
<tr>
<td>PDE</td>
<td>partial differential equation</td>
</tr>
<tr>
<td>PE</td>
<td>processing element</td>
</tr>
<tr>
<td>rms</td>
<td>root of mean square</td>
</tr>
<tr>
<td>SRA</td>
<td>strong Reynolds analogy</td>
</tr>
<tr>
<td>TKE</td>
<td>turbulent kinetic energy</td>
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Abstract

The effects of Mach number and wall temperature on the turbulence structure of a supersonic boundary layer have been investigated employing an extended temporal direct numerical simulation (ETDNS) method. The ETDNS method has allowed to describe with precision and for the first time the turbulence structure of highly supersonic boundary layers, which no experimental technique has achieved yet. A $M_\infty = 4.5$ boundary layer over a strongly cooled wall displays roughly the same turbulence structure as over a nearly adiabatic wall, however with a lower fluctuation level. The intrinsic effects of compressibility on turbulence statistics are confirmed to be small even up to a Mach number of 6. At high Mach numbers ($M_\infty \gtrsim 5$), a region of higher turbulent activity appears near the mid boundary-layer, and the validity of Morkovin’s hypothesis is restricted.

Kurzfassung

Mit einer neuen zeitlichen DNS-Methode (ETDNS) sind die Machzahl- und Wandtemperatureffekte auf die Turbulenzstruktur einer Überschallgrenzschicht untersucht worden. Zum ersten Mal konnte mit Hilfe der ETDNS Methode die Turbulenzstruktur von Grenzschichten im hohen Überschallbereich mit Präzision beschrieben werden, was bis jetzt keiner experimentellen Technik gelungen ist. Die Grenzschicht an einer stark gekühlten Wand bei $M_\infty = 4.5$ weist ungefähr die gleiche Turbulenzstruktur auf wie an einer quasi-adiabaten Wand, jedoch mit geringeren turbulenten Fluktuationen. Kompressibilitätseffekte wie Druckdilatationskorrelation und Dilatationsdissipation bleiben klein sogar bei $M_\infty = 6$. Bei hoher Machzahl ($M_\infty \gtrsim 5$) entsteht etwa in der Mitte der Grenzschicht ein Bereich erhöhter turbulenten Aktivität, und die Morkovinsche Hypothese ist nur noch begrenzt gültig.
Chapter 1

Introduction

Fluid mechanics is plagued by the difficulty that man’s ability to write the governing equations of motion far outruns his ability to solve them. This point is an especially annoying handicap in the case of turbulent flows. Numerous famous physicists, including Lamb, Heisenberg, Sommerfeld, Einstein and Feynman, are said to have recognized that turbulence is the last great unsolved problem of classical physics. Turbulent flows have been investigated for more than a century, but no general approach to the solution of problems in turbulence exists. The equations of motion have been analyzed in great details, but it is still almost impossible to make accurate quantitative predictions without relying heavily on empirical data. Statistical studies of the equations of motion always lead to a situation in which there are more unknowns than equations. This is the closure problem of turbulence theory: one has to make (very often ad hoc) assumptions to make the number of equations equal the number of unknowns.

The history of research in turbulent compressible flows is somewhat checkered, in that changes in national and international priorities have had a large impact on the continuity of effort. The high level of activity that lasted from the mid-forties to the mid-sixties of the twentieth century was largely driven by the wish to fly at supersonic speeds, and the need to solve the hypersonic re-entry problem. Once these aims were met, the general level of urgency diminished considerably, and further efforts became severely reduced. Recently, we saw another upsurge in activity, driven mainly by a new set of national priorities, such as the desire to fly at hypersonic speeds and the projected need for a low-cost supersonic transport aircraft. To reach those aims, significant levels of new research will be required to improve fuel efficiency, reduce pollution and minimize noise. A better understanding of compressibility on turbulence will have a crucial impact on the development of answers to these engineering challenges.
In this work, we focus our attention on turbulent flat-plate boundary layers in the high supersonic regime. The geometry might appear excessively simple, but the presence of the wall, the associated strong shear and anisotropy make the problem complicated enough. The aim of this work is to investigate compressible boundary layers by means of direct numerical simulation (DNS) in order to see and then describe the phenomena taking place in these flows.

There is already a respectable amount of experimental data available, covering a broad range of Reynolds and Mach numbers, and a large part of it has been collected, sorted and commented by Fernholz & Finley [22, 23, 24]. More recently, Dussauge et al. [17] reviewed the state of the art of experimental knowledge in turbulent boundary layers. Although, on the one hand, the mean-flow behavior has been precisely documented, the turbulence statistics on the other hand still suffer from a relatively large scatter [79]. For high Mach number flows, non-intrusive measuring techniques with flow seeding can not be employed as the particles' inertia becomes so large that the tracers can no longer fulfill their role (i.e. being transported by the flow as massless particles). The alternative with probes (Pitot, hot wires) inserted into the flow is also awkward, as the slenderness required to disturb the flow as little as possible can hardly be accommodated to a certain stiffness needed to resist the huge aerodynamic loads. Besides, when the local Mach number is higher than one, a shock can form in front of the probe so that some additional post-processing is needed to recover the data of the corresponding undisturbed flow.

Thus, the direct numerical simulation appears as a valuable complement to the experimental techniques in order to give an accurate time and space representation of these flows. The advantage of the DNS over other numerical simulation techniques (Reynolds averaged Navier-Stokes equations or large-eddy simulations) is that it requires no turbulence or subgrid-scale model, as the grid spacing is chosen fine enough to resolve all relevant scales. Still the DNS remains expensive and suffers from many limitations in terms of geometric complexity and Reynolds number. The restrictions are linked to the capacities (speed and memory) of the available computer systems, whose continual evolution allows to always broaden the investigation field of the DNS. However, compressible flows in or over complex geometries at high Reynolds numbers are not likely to be simulated by DNS in a foreseeable future. Nevertheless, the study of geometrically simpler problems at low to moderate Reynolds number has its place in a logic of increasing complexity,
where some basic issues are first investigated separately before the knowledge gained thereby is employed to grapple with higher-level problems.

The history of DNS as a tool in turbulence research has been recently reviewed by Moin & Mahesh [51]. After its birth with the $32^3$ computation of isotropic turbulence at low Reynolds number by Orszag & Patterson [56] in 1972, the DNS was first developed for incompressible flows. Some major steps in this evolution are the work of Rogallo [63] on homogeneous turbulence subjected to mean strain, the plane channel flow simulation of Kim et al. [37] and the flat-plate boundary layer simulation of Spalart [76]. Recently, some reasonably complex flows have been computed, like the flow over a backstep [44] and a flat-plate boundary layer separation [55].

The problem of compressible turbulent flows was tackled more recently. The early eighties saw DNS of homogeneous compressible turbulence being initiated, but only a decade later was a serious study of isotropic and sheared homogeneous compressible turbulence undertaken [20, 69, 8]. A DNS of high-speed turbulent mixing layers was performed by Vreman et al. [84]. Wall-bounded flows such as the compressible channel [14] and the turbulent boundary layer [29, 60, 28] have also only recently been attempted, as well as the ramp flow [2]. The specificity of the simulations presented here is that they venture into a Mach number and Reynolds number range which have not been touched yet by DNS, though the Reynolds numbers reached are still smaller than those of "real" industrial applications.

Smits & Dussauge [73] recognize that the description we have at present of the two-dimensional incompressible flat-plate boundary layer is reasonably complete. At supersonic speed however, we are only starting to develop a similar description of the boundary layer structure, and the picture is not nearly so complete as in the case of incompressible flows.

Supersonic boundary layers have been reviewed e.g. by Morkovin [52, 53], Bradshaw [10], Smits [72], Lele [46], Spina et al. [79] and Smits & Dussauge [73]. As computer simulations are still sparse, most of the knowledge is based on experimental information.

A density gradient caused by the dissipative heating near the no-slip wall is the primary effect of an increasing free-stream Mach number $M_\infty$ in a zero-pressure gradient flat-plate supersonic boundary layer. It is broadly agreed upon that the direct effects of compressibility on wall turbulence are small for free-stream Mach numbers less than about 5 [72]. Furthermore, some of the most noticeable differences between subsonic and supersonic boundary layers may be attributed to the variation of fluid properties across
the layer. This is in essence Morkovin's hypothesis [52, 9].

When the mean streamwise velocity is plotted in classic inner- and outer-layer coordinates, it does not follow the familiar incompressible scaling laws for these regions (logarithmic law, law of the wake [73]). However, a modified scaling that accounts for the fluid-property variations collapses much of the existing compressible mean-velocity data onto the "universal" incompressible distribution. This velocity scaling, the van Driest transform [83], has become an accepted standard. It is however still unclear what exact value the von Kármán constant employed in the logarithmic law assumes [23, 75, 57].

If the longitudinal velocity fluctuations are normalized by the friction velocity, there is a clear decrease of the fluctuation level with increasing free-stream Mach number $M_\infty$ [24]. However, when the streamwise normal Reynolds stress $\rho u'w'$ is normalized by the wall shear stress, the data exhibit some degree of similarity, particularly in the outer layer. This formulation of the velocity fluctuations indicates a certain success of the scaling proposed by Morkovin [52] to account for the mean density variation. The distribution of the streamwise normal Reynolds stress for experimental compressible data is in fair agreement with the incompressible results of Klebanoff [38], except near the wall where the supersonic measurements are subject to considerable uncertainty. Morkovin's scaling appears to be appropriate up to a Mach number of at least 5. At $M_\infty = 6.7$, measurements by Owen et al. [59] show damped turbulent fluctuations, particularly near the wall. This is however for cold-wall conditions and may indicate the stabilizing effect of wall cooling [79] rather than a Mach-number effect.

Measurements of the spanwise $v'^2$ and wall-normal $w'^2$ velocity fluctuations are less common than those of $u'^2$ and data exhibit more scatter, so that conclusions are less certain. In contrast to the streamwise turbulent intensity, both distributions appear to increase slightly with increasing Mach number [24] and Morkovin's scaling does not collapse the data. Sandborn [65] reviewed available data of the zero-pressure gradient Reynolds shear stress $\rho u'w'$. He constructed a "best fit" of normalized shear-stress profiles $\tau/\tau_w$ from integrated mean-flow data taken by several different research groups over a wide Mach-number range ($2.5 < M_\infty < 7.2$) for adiabatic and cold walls. The data indicate a nearly universal shear-stress profile that is in excellent agreement with the incompressible measurements of Klebanoff [38]. However, subsequent Reynolds stress measurements (e.g. Robinson
[61], Smits & Muck [74], Donovan & Spina [16]) have exhibited only a modest agreement with Sandborn's best fit and the incompressible distribution. The agreement is limited to the outer layer, with tremendous scatter in the inner layer, and most profiles do not tend toward $\tau/\tau_w = 1$ near the wall. The data in the inner layer do not scale with $z^+ = zu_*/\nu_w$, probably because of the difficulties with the measurements. Lele [46] finds that present measurements allowing the compressibility effects on turbulence to be isolated are very limited.

The strong Reynolds analogy (SRA), first identified as such by Morkovin [52] but primarily due to Young [87], relates the temperature fluctuations to the streamwise velocity fluctuations, assuming zero total temperature fluctuations. It is widely used for the reduction of experimental data and the comparison of compressible and incompressible results [79]. Morkovin [52] and Gaviglio [27] tested the time-averaged form of the SRA and found that the correlation coefficient $R_{u''T''}$ between $u''$ and $T''$ is not $-1$ as predicted but is closer to $-0.8$. However, even if the total temperature fluctuations were seen to be not negligible, it was shown that results derived from such an assumption still represent good approximations [18, 71].

The SRA and the Morkovin hypothesis are staples of boundary-layer analysis at moderate Mach numbers. However, an upper Mach number limit must exist on the applicability of these simplifying assumptions [79].

Coleman et al. [14] performed direct numerical simulations of turbulent supersonic channel flows at Mach numbers 1.5 and 3 with cooled isothermal walls. They found that the isothermal-wall flow is strongly influenced by sharp gradients of mean density and temperature that occur near the walls. In these regions, the high $\rho$ and $T$ fluctuations are mostly of a non-acoustic nature, primarily the result of solenoidal passive mixing across a mean gradient. The results of Coleman et al. agree in many ways with the incompressible DNS data of Kim et al. [37] when properly scaled to account for mean property variations.

In their extensive review of supersonic flow data, Fernholz & Finley [23, 24] list only a few experiments where heat transfer is important, and these cases are confined to cooled walls. Nevertheless, they conclude that both the logarithmic law of the wall and the outer law agree satisfactorily with measurements in supersonic turbulent boundary layers with zero-pressure gradient along isothermal walls. Laderman [42] and Laderman & Demetriades [43] investigated fully developed Mach 3 turbulent boundary layers with negligible pressure gradient over adiabatic and cooled walls. They reported that,
for moderate heat-transfer rates, the structure of their boundary layers was unaffected by heat transfer to the wall. Furthermore, turbulent transport properties deduced from the mean flow were found to be in good agreement with results for compressible adiabatic flows. Their results support Sandborn’s earlier theory [65] that when expressed in the form $\tau/\tau_w$ versus $z/\delta_0$, the shear stress distribution is essentially independent of Mach number and heat transfer. The measurements carried out by Horstman & Owen [31] in a Mach 7.2 turbulent cold-wall boundary layer revealed that the turbulent property distributions extracted from mean-flow data (such as mixing-length, eddy-viscosity and turbulent Prandtl number distributions) were in good agreement with earlier incompressible and adiabatic results.

One of the objectives of this work was to gain experience in DNS of turbulence on a massively parallel computer by parallelizing an existing code and porting it onto such an architecture, and to compare the performance with other parallel computer designs. Then, using this powerful computational tool, the potential of the extended temporal DNS (ETDNS) method was to be investigated for larger simulation domains and extended simulation times (compared to the serial version of the code). The other objective of this research was to establish an accurate database which enables a better understanding of the physics of supersonic turbulent boundary layers, particularly by studying carefully the influence of the wall temperature and of the Mach number (compressibility). Also, the validity at high Mach numbers of the Morkovin hypothesis, the strong Reynolds analogy and the van Driest transformation could be evaluated, along with the relevance of some turbulence models in supersonic wall-bounded flows.

This work is structured as follows. The modeling principle and the related governing equations are described in chapter 2. The numerical aspects of the code are then presented in chapter 3. In chapter 4 the explicit parallelization of the employed code and optimization for the CRAY T3D platform are detailed. Chapter 5 gives an overview of the simulation results with the main parameters and the relevant integral values, together with the description of some experimental cases used for comparison. A detailed description of the results follows in chapter 6 for the wall-temperature effects and in chapter 7 for the influence of the Mach number. Some additional issues pertaining to all presented simulations are then discussed in chapter 8. Chapter 9 summarizes the conclusions of this study and gives some recommendations for future work.
Chapter 2

Physical model

Throughout this work, dimensionless quantities will be used. Dimensional quantities are marked with an asterisk "*".

Some physical assumptions have to be made for the investigated fluid flow. The turbulent flow is considered as a continuum phenomenon where the smallest turbulent scales of motion are very much larger than molecular scales of motion [81]. The relevant molecular length scale is the mean free-path $\lambda^*$, while the Kolmogorov length scale $\eta^*$ represents the size of the smallest eddies in a turbulent flow. The ratio of those two reference lengths $\lambda^*/\eta^*$, defined as the microstructure Knudsen number [81], is

$$\frac{\lambda^*}{\eta^*} \sim \frac{M_t}{Re_t^{1/4}},$$  \hspace{1cm} (2.1)

where $M_t$ is the turbulence Mach number and $Re_t = \sqrt{\frac{\bar{u}' \bar{u}'}{\nu}} \frac{\delta_0}{\nu}$ the turbulence Reynolds number. In the investigated cases, the magnitude of the microstructure Knudsen number is typically 0.03 ... 0.04, so that the continuum assumption is justified.

Thermodynamic equilibrium is considered as a good approximation even if, strictly speaking, a viscous fluid in motion is technically not in equilibrium [85] (whereas the deviations are negligible at normal densities, which applies here). The considered fluid follows the perfect-gas law and has constant specific heats ($c_p^*$, $c_v^*$). Chemical reactions of any sort are neglected.

According to Stokes’s hypothesis, the bulk viscosity is neglected [70]. The considered fluid is assumed to be Newtonian, so that the functional relationship between the shear and the strain rate is linear. The proportionality factor, the dynamic viscosity $\mu$, is set to be a function of the temperature only, according to Sutherland’s law. Furthermore, Fourier’s law of heat conduction is postulated, where the heat flux is proportional to the temper-
ature gradient. Finally, the ratio of viscosity to thermal conductivity, the Prandtl number $Pr$, is assumed to be constant.

2.1 Modeling principle

In a turbulent flat-plate equilibrium boundary-layer flow with zero-pressure gradient, the mean flow changes on a “slow” scale in the streamwise direction whereas turbulent fluctuations vary on a “fast” scale (this two-scale analysis was first applied successfully to incompressible boundary layers by Spalart [76]). Following this idea, one can consider the mean-flow quantities as global quantities, carrying information in the streamwise direction, while turbulent quantities are more local, being generated and dissipated within a shorter time and smaller space.

In the present work, the turbulent quantities are calculated locally with a temporal DNS (TDNS) approach, while at the same time the global spatial evolution of the mean flow is set to obey parabolized steady Reynolds-averaged Navier-Stokes equations. We will refer to this procedure as an extended TDNS or ETDNS. The ETDNS approach was developed in the early 1990s and employed for the first time by Guo and Adams [29, 30]. The basic numerical modeling principle follows the TDNS approach, as described by Kleiser & Zang [39], where the mean flow is assumed to be locally parallel and to develop in time. The computational domain is thus chosen relatively short so that the mean-flow change in the streamwise direction can be neglected. Yet the domain is also required to be large enough to allow turbulent fluctuations to decorrelate sufficiently.

In a classical TDNS, the assumption of streamwise periodicity leads to a non-stationary mean-flow behavior as streamwise mean-flow gradients are omitted. In the extended TDNS version, the mean-flow growth is taken into account to some extent through the addition of forcing terms to the basic equations. In order to be able to reconstruct the mean-flow upstream history, a marching scheme is applied in which the computational domain is moved stepwise downstream during the simulation. At each spatial station, the local solution of the flow is integrated in time. When a satisfactory statistically steady state is reached, local mean-flow profiles are stored and the computational domain is moved one step downstream to a new station where the time-integration starts again, see figure 2.1. Thus, using the mean-flow information of the last stations, it is possible to calculate the local
2.2 Governing equations

The equations solved at a fixed spatial station are the compressible Navier-Stokes equations in conservative form

\[
\frac{\partial \mathbf{U}}{\partial t} = \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \frac{\partial \mathbf{H}}{\partial z} + \mathbf{Z}_0 + \mathbf{Z}_1 + \mathbf{Z}_c.
\]

(2.2)

The Cartesian coordinate system is illustrated in figure 2.1. For notational

Figure 2.1: Principle of the extended temporal DNS (ETDNS).
convenience we use synonymously \( \{x, y, z\} \equiv \{x_1, x_2, x_3\} \) and \( \{u, v, w\} \equiv \{u_1, u_2, u_3\} \). The vector \( \mathbf{U} \) contains the conservative variables \( \{\rho, \rho u, \rho v, \rho w, E\} \). The density \( \rho \) is normalized with \( \rho^*_\infty \), the three velocity components \( u, v, w \) with \( u^*_\infty \). \( E \) is the total energy defined as

\[
E = \frac{1}{\gamma - 1} p + \frac{\rho}{2} (u^2 + v^2 + w^2),
\]

where \( \gamma \) is the ratio of specific heats (assumed to be constant) and \( p \) is the static pressure normalized with \( \rho^*_\infty u^*_\infty \). The flux vectors \( \mathbf{F}, \mathbf{G} \) and \( \mathbf{H} \) are given by

\[
\mathbf{F} = \begin{bmatrix}
-\rho u \\
-\rho u^2 - p + \tau_{xx} \\
-\rho uv + \tau_{xy} \\
-\rho uw + \tau_{xz} \\
-\mathcal{u}(E + p) - q_x + u\tau_{xx} + v\tau_{xy} + w\tau_{xz}
\end{bmatrix}, \tag{2.4}
\]

\[
\mathbf{G} = \begin{bmatrix}
-\rho v \\
-\rho uv + \tau_{xy} \\
-\rho v^2 - p + \tau_{yy} \\
-\rho vw + \tau_{yz} \\
-\mathcal{v}(E + p) - q_y + u\tau_{xy} + v\tau_{yy} + w\tau_{yz}
\end{bmatrix}, \tag{2.5}
\]

\[
\mathbf{H} = \begin{bmatrix}
-\rho w \\
-\rho uw + \tau_{xz} \\
-\rho vw + \tau_{yz} \\
-\rho w^2 - p + \tau_{zz} \\
-\mathcal{w}(E + p) - q_z + u\tau_{xz} + v\tau_{yz} + w\tau_{zz}
\end{bmatrix}, \tag{2.6}
\]

where the viscous stresses are

\[
\tau_{ij} = \frac{\mu}{Re} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right), \tag{2.7}
\]

for \( i, j = 1, 2, 3 \). The viscosity \( \mu \) is computed with Sutherland’s law

\[
\mu(T) = T^2 \frac{1 + Su}{T + Su} \tag{2.8}
\]
and normalized with $\mu^*_\infty$. The constant $Su$ is given by $Su = 110.4K/T^*_\infty$ and the computational Reynolds number is

$$Re = \frac{\rho^*_\infty u^*_\infty \delta^*_\infty_{lam}}{\mu^*_\infty},$$

(2.9)

where $\delta^{*}_{lam}$ is the displacement thickness of the initial laminar flow field, which became, after its transition, the initial-condition flow field for the turbulent simulation, see section 2.5. The different thicknesses used in this work are defined as follows

- boundary-layer thickness: $\bar{u}(z = \delta_0) = 0.995 u_\infty$, (2.10)
- compressible thickness: $\bar{u}^+_V (z = \delta_c) = 0.9999 u^+_V$, (2.11)
- displacement thickness: $\delta_1 = \int_0^\infty (1 - \frac{\rho \bar{u}}{\rho_\infty u_\infty}) dz$, (2.12)
- momentum thickness: $\delta_2 = \int_0^\infty \frac{\rho \bar{u}}{\rho_\infty u_\infty} (1 - \frac{\bar{u}}{u_\infty}) dz$, (2.13)

where $\bar{u}^+_V$ is defined in equation (6.4). The ratio of $\delta_1$ to $\delta_2$ is the form factor $H_{12}$ ($H_{12} = \delta_1/\delta_2$). An overline $\bar{\bullet}$ denotes a Reynolds-averaged quantity and a tilde $\tilde{\bullet}$ a Favre-averaged quantity. The Favre or mass average of a quantity $f$ is computed as $\bar{f} = \rho \bar{f}/\bar{\rho}$. A single prime $'\bullet'$ indicates a fluctuation with respect to a Reynolds average, a double prime $''\bullet''$ a fluctuation with respect to a Favre average.

The heat-flux vector $\mathbf{q}$ is given by

$$q_i = -\frac{\mu/Re}{(\gamma - 1)M^2_\infty Pr} \frac{\partial T}{\partial x_i}. $$

(2.14)

The Prandtl number $Pr = \mu^* c^*_p/\lambda^*$ is assumed to be constant. The specific heat at constant pressure is $c^*_p$ and $\lambda^*$ represents the thermal conductivity.

The pressure $p$ can be calculated from the conservative variables and the temperature $T$ (normalized with $T^*_\infty$) is obtained with the perfect-gas law

$$p\gamma M^2_\infty = \rho T. $$

(2.15)

The different forcing terms $Z_0$, $Z_1$ and $Z_c$ are described in section 2.4.
2.3 Boundary conditions

In the streamwise and spanwise directions

The space of approximation functions to the solution of the governing equations is restricted to its 2-periodic subset (in $x$ and $y$). Thus the periodic boundary conditions are implicitly satisfied by the Fourier-expansion formulation in $x$ and $y$ (see chapter 3).

At the wall

At the wall ($z = 0$), Dirichlet boundary conditions for the velocity and temperature are given. The wall is set to be isothermal ($T_w = \text{const}$) and the no-slip condition is enforced ($u_w = v_w = w_w = 0$). Besides, the wall-normal momentum balance is enforced at the wall whenever a wall-normal pressure gradient is computed, by requiring that the discrete pressure gradient satisfies

$$\frac{\partial p}{\partial z} \bigg|_w = \frac{\partial \tau_{x z}}{\partial x} \bigg|_w + \frac{\partial \tau_{y z}}{\partial y} \bigg|_w + \frac{\partial \tau_{zz}}{\partial z} \bigg|_w,$$

using the discrete representations of the stress-tensor components. This allows to compute $\partial p/\partial z$, which is a sensitive value, with a better accuracy.

At the upper truncation plane

Non-reflecting conditions are implemented using a characteristic formulation for the hyperbolic terms, provided that the viscous terms are negligibly small [82]. For this condition to be satisfied, care must be taken that the computational domain height $z_{max}$ is sufficiently larger than the boundary-layer thickness $\delta_0$. Thus, at the upper or free-stream boundary, the parabolic part of the Navier-Stokes equations can be assumed to vanish. For the remaining reduced hyperbolic system, the non-reflecting boundary conditions of Thompson [82] are used. Defining the characteristic variables

$$Q := \left[ \begin{array}{c} \rho - \frac{p}{c^2} \\ u \\ v \\ \frac{p}{2c^2} + \frac{\rho w}{2c} \\ \frac{p}{2c^2} - \frac{\rho w}{2c} \end{array} \right], \quad (2.16)$$
where \( c \) is the local speed of sound, the boundary conditions can be written as the variation of \( Q \)

\[
\delta Q_i = \begin{cases} 
\frac{\partial Q_{i+1}}{\partial t} + \lambda_i \frac{\partial Q_{i+1}}{\partial z} = 0 & , \lambda_i \geq 0 \\
0 & , \lambda_i < 0 
\end{cases} \quad (i = 1, \ldots, 5)
\]  

(2.17)

where \( \lambda_i \) is an eigenvalue of the local flux Jacobian of the reduced hyperbolic system. Thus the boundary condition causes the characteristic variables along the incoming characteristic lines \( \lambda_i < 0 \) to be constant. It means that (perturbation) waves can not enter the computational domain, but can leave it without reflection. Further details can be found in appendix A.

### 2.4 Forcing terms

As illustrated in figure 2.1, the ETDNS method approximates the spatial development of a boundary layer in a discrete way, sampling the flow at a sequence of streamwise stations \( X_n \) \((n > 0)\), where \( X \) represents the slow streamwise coordinate. Through this sequence of stations the mean boundary layer evolves slowly, according to parabolized steady Reynolds-averaged Navier-Stokes (PRANS) equations. The parabolization is carried out by setting to zero all terms containing second derivatives \( \partial^2/\partial X^2 \) after thorough expansion with the chain rule. At each station, the full unsteady Navier-Stokes equations are solved within the computational domain, augmented by forcing terms which ensure that the mean flow is a solution of the PRANS equations at this station.

For clarity, the derivation of the forcing terms for the ETDNS approach is first demonstrated for an incompressible flow. The flow field can be decomposed as \( \mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}' \), where \( \bar{\mathbf{u}} \) represents the mean flow and \( \mathbf{u}' \) the remaining fluctuating part. The governing equations for \( \bar{\mathbf{u}} \) are the Reynolds-averaged Navier-Stokes equations

\[
\nabla \cdot \bar{\mathbf{u}} = 0
\]

(2.18)

\[
\nabla \cdot (\bar{\mathbf{u}} \otimes \bar{\mathbf{u}}) = -\nabla \bar{p} + \frac{1}{Re} \nabla^2 \bar{\mathbf{u}} - \nabla \cdot (\mathbf{u}' \otimes \mathbf{u}')
\]

(2.19)

where \( \bar{\mathbf{u}}' \otimes \bar{\mathbf{u}}' \) are the Reynolds stresses and the overline represents a time-averaged quantity. In a flat-plate boundary layer with zero-pressure gradient, \( \bar{\mathbf{u}} \) varies slowly in the streamwise direction, so that the governing
equation (2.19) can be parabolized by dropping the X-derivatives in the diffusive terms

\[ \nabla \cdot \mathbf{u} = 0 \]  \hspace{1cm} (2.20)

\[ \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) = -\nabla \bar{p} + \frac{1}{Re} \nabla_{P}^{2} \mathbf{u} - \nabla \cdot (\mathbf{u}' \otimes \mathbf{u}') \]  \hspace{1cm} (2.21)

where \( \nabla_{P} = \{0 , \partial/\partial y , \partial/\partial z \} \).

In a conventional TDNS approach, the full Navier-Stokes equations are solved, however with streamwise periodic boundary conditions. In the case of a zero-pressure gradient boundary layer, one can assume \( \mathbf{u} \) to be homogeneous in the \((x,y)\) plane. Thus, with the ergodicity principle, ensemble-averaged statistics are computed from plane averages in the homogeneous directions \( x \) and \( y \). The equations governing the mean flow in a TDNS are then

\[ \nabla_{P} \cdot \bar{\mathbf{u}} = 0 \]  \hspace{1cm} (2.22)

\[ \frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla_{P} \cdot (\bar{\mathbf{u}} \otimes \bar{\mathbf{u}}) = -\nabla_{P} \bar{p} + \frac{1}{Re} \nabla_{P}^{2} \bar{\mathbf{u}} - \nabla_{P} \cdot (\bar{\mathbf{u}}' \otimes \bar{\mathbf{u}}') \]  \hspace{1cm} (2.23)

Note that \( \bar{\mathbf{u}} \) is here a function of time and an overline denotes a quantity which has been averaged spatially over \( x \) and \( y \). If we compare equations (2.20) and (2.21) with equations (2.22) and (2.23), we see that following terms are missing on the right-hand side of equations (2.22) and (2.23)

\[ Z_{0s} = \begin{bmatrix} -\frac{\partial \bar{u}}{\partial X} \\ -\frac{\partial \bar{w}}{\partial X} - \frac{\partial \bar{p}}{\partial X} - \frac{\partial \bar{w}' \bar{w}'}{\partial X} \\ -\frac{\partial \bar{u}' \bar{w}'}{\partial X} - \frac{\partial \bar{w}' \bar{w}'}{\partial X} \\ -\frac{\partial \bar{u}' \bar{w}'}{\partial X} - \frac{\partial \bar{w}' \bar{w}'}{\partial X} \end{bmatrix} \]  \hspace{1cm} (2.24)

Note that the streamwise variation of the Reynolds stresses is included in the term \( Z_{0s} \). Equations (2.22) and (2.23) with \( Z_{0s} \) added on their right-hand side constitute a transient problem of the equations (2.20) and (2.21) and both systems converge to the same solution if \( \partial \bar{\mathbf{u}}/\partial t \) goes to zero. At each spatial station \( X_{n} \), the solution of the full equation (2.22) and (2.23) with \( Z_{0s} \) added is integrated in time until a statistically steady state is reached. The solution is then marched downstream to the next spatial station \( X_{n+1} \).

The length of the spatial step is chosen typically as a few times (\( \sim 2 \ldots 7 \) times) the length of the computational domain, which corresponds to 4 \ldots 10
boundary-layer thicknesses $\delta_0$. This is on the one hand big enough to avoid an overlap of the computational domains at the different stations, and on the other hand sufficiently short so that the local boundary layer does not become too thick and still fits in the computational box. Because of the slow streamwise flow development, discretization errors are negligible when the above-mentioned step size is employed.

The marching scheme allows thus to compute the slow streamwise derivatives of the mean quantities that a classical TDNS method can not represent. For the approximation of these derivatives, a second-order backward-difference formula is used, which is for a variable $f$ at station $n$

$$
\frac{\partial f}{\partial X} \bigg|_n = \frac{1}{X_n - X_{n-1}} \left( \frac{1 + 2\omega_n}{1 + \omega_n} f_n \right.
\left. - (1 + \omega_n) f_{n-1} + \frac{\omega_n^2}{1 + \omega_n} f_{n-2} \right),
$$

(2.25)

where $\omega_n = (X_n - X_{n-1})/(X_{n-1} - X_{n-2})$. During the first three spatial steps a backward differentiation formula of first order is employed, in which only stations $n$ and $n - 1$ are used

$$
\frac{\partial f}{\partial X} \bigg|_n = \frac{1}{X_n - X_{n-1}} (f_n - f_{n-1}).
$$

(2.26)

The forcing term $Z_{0g}$ takes into account the effects of mean-flow non-parallelity on the mean-flow itself, while the interaction of mean-flow non-parallelity with the fluctuating flow part has not been accounted for yet.

Consider now the nonlinear term $\partial (u_i u_j)/\partial x_g$ using again the decomposition into the mean and fluctuating part $u_k = \bar{u}_k + u'_k$. For clarity, a general streamwise coordinate $x_g$ is introduced, which is valid for all scales in the streamwise direction. In order to take into account the slow and fast variation in the streamwise direction, we write formally $\partial/\partial X$ for “slow” derivatives, see equations (2.25) and (2.26), and $\partial/\partial x$ for “fast” derivatives. The following is then valid

$$
\frac{\partial \bar{u}_i}{\partial x} = 0, \quad \frac{\partial u'_i}{\partial x} = 0,
$$

and formally

$$
\frac{\partial u_i}{\partial x_g} = \frac{\partial \bar{u}_i}{\partial X} + \frac{\partial u'_i}{\partial x}.
$$

(2.27)
The nonlinear term becomes
\[
\frac{\partial (u_i u_j)}{\partial x_g} = \frac{\partial}{\partial x_g} \left( (\bar{u}_i + u_i')(\bar{u}_j + u_j') \right) \\
= \frac{\partial \bar{u}_i \bar{u}_j}{\partial X} + \bar{u}_i \frac{\partial u_j'}{\partial x} + u_j \frac{\partial \bar{u}_i}{\partial X} + u_i' \frac{\partial \bar{u}_j}{\partial X} + \bar{u}_j \frac{\partial u_i'}{\partial x} + \frac{\partial u_i' u_j'}{\partial x}, \quad (2.28)
\]
which can be rearranged as
\[
\frac{\partial (u_i u_j)}{\partial x_g} = \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial X} + u_j' \frac{\partial \bar{u}_i}{\partial X} + u_i \frac{\partial \bar{u}_j}{\partial X} + \frac{\partial (u_i u_j)}{\partial x}, \quad (2.29)
\]
where the term on the left-hand side of equation (2.29) belongs to the global Navier-Stokes equations. While term 1° is part of \(Z_{0g}\) and term 3° is solved locally in the Navier-Stokes equations with a TDNS formulation, term 2° representing the interaction of mean-flow non-parallelity and local fluctuations is missing. Applying the same analysis for all relevant terms, we obtain the following expression which is then added to the locally solved Navier-Stokes equations
\[
Z_{1s} = \begin{bmatrix}
0 \\
-2(u - \bar{u}) \frac{\partial \bar{u}}{\partial X} \\
-(u - \bar{u}) \frac{\partial \bar{v}}{\partial X} - (v - \bar{v}) \frac{\partial \bar{u}}{\partial X} \\
-(u - \bar{u}) \frac{\partial \bar{w}}{\partial X} - (w - \bar{w}) \frac{\partial \bar{u}}{\partial X}
\end{bmatrix}. \quad (2.30)
\]
Note that \(Z_{1s}\) only acts on the governing equation for \(u' = u - \bar{u}\).

For compressible boundary-layer flows, the forcing terms are derived in the same manner. The \(Z_0\) compressible forcing term is now
\[
Z_0 = \frac{\partial}{\partial X} \begin{bmatrix}
-\rho u \\
-\rho u^2 - \bar{p} + \bar{\tau}_{xx} \\
-\rho u \bar{v} + \bar{\tau}_{xy} \\
-\rho u \bar{w} + \bar{\tau}_{xz} \\
-u(E + p) - \bar{q}_x + u \bar{\tau}_{xx} + \bar{v} \bar{\tau}_{xy} + \bar{w} \bar{\tau}_{xz}
\end{bmatrix} + Z_m \quad (2.31)
\]
Forcing terms

The term $Z_m$, which contains further terms missing in the compressible equivalent of (2.23), is small compared to $Z_0$ but is nevertheless retained

$$Z_m = \frac{1}{Re} \begin{bmatrix}
0 \\
\frac{4}{3} \frac{\partial \bar{\mu}}{\partial X} \frac{\partial \bar{u}}{\partial X} + \frac{\partial}{\partial y} \left( \bar{\mu} \frac{\partial \bar{v}}{\partial X} \right) + \frac{\partial}{\partial z} \left( \bar{\mu} \frac{\partial \bar{w}}{\partial X} \right) \\
\frac{\partial \bar{\mu}}{\partial X} \frac{\partial \bar{v}}{\partial X} - \frac{2}{3} \frac{\partial}{\partial y} \left( \bar{\mu} \frac{\partial \bar{u}}{\partial X} \right) \\
\frac{\partial \bar{\mu}}{\partial X} \frac{\partial \bar{w}}{\partial X} - \frac{2}{3} \frac{\partial}{\partial z} \left( \bar{\mu} \frac{\partial \bar{u}}{\partial X} \right) \\
\frac{1}{(\gamma-1)M_\infty^2 Pr} \frac{\partial \bar{\mu}}{\partial X} \frac{\partial \bar{T}}{\partial X} + \frac{4}{3} \mu \left( \frac{\partial \bar{u}}{\partial X} \right)^2 + \frac{4}{3} \bar{\mu} \frac{\partial \bar{u}}{\partial X} \frac{\partial \bar{u}}{\partial X} + \bar{\mu} \left( \frac{\partial \bar{v}}{\partial X} \right)^2 + \bar{\mu} \frac{\partial \bar{v}}{\partial X} \frac{\partial \bar{v}}{\partial X} + \frac{\partial}{\partial y} \left( \mu \bar{\mu} \frac{\partial \bar{u}}{\partial X} \right) - \frac{2}{3} \frac{\partial}{\partial y} \left( \mu \bar{\mu} \frac{\partial \bar{u}}{\partial X} \right) + \frac{\partial}{\partial z} \left( \mu \bar{u} \frac{\partial \bar{w}}{\partial X} \right) - \frac{2}{3} \frac{\partial}{\partial z} \left( \mu \bar{u} \frac{\partial \bar{w}}{\partial X} \right)
\end{bmatrix}. \quad (2.32)$$

As we assume here a zero-pressure gradient flat-plate boundary layer, the term $\partial \bar{p} / \partial X$ is set to zero. The term $Z_1$ is given by

$$Z_1 = \begin{bmatrix}
-\rho \frac{\partial \bar{u}}{\partial X} - u \frac{\partial \bar{p}}{\partial X} + \frac{\partial \bar{u}}{\partial X} \\
-(u - \bar{u}) \frac{\partial \rho \bar{u}}{\partial X} - (\rho u - \bar{p} u) \frac{\partial \bar{u}}{\partial X} \\
-(u - \bar{u}) \frac{\partial \rho \bar{v}}{\partial X} - (\rho v - \bar{p} v) \frac{\partial \bar{v}}{\partial X} \\
-(u - \bar{u}) \frac{\partial \rho \bar{w}}{\partial X} - (\rho w - \bar{p} w) \frac{\partial \bar{w}}{\partial X} \\
-(u - \bar{u}) \frac{\partial (\bar{E} + \bar{p})}{\partial X} - (E + p - \bar{E} - \bar{p}) \frac{\partial \bar{u}}{\partial X}
\end{bmatrix}. \quad (2.33)$$

Both streamwise and spanwise spatial averaging can be performed for the quantities with an overbar at $X_n$. At the stations $X_{n-1}$ and $X_{n-2}$, time averaging is also implemented, which allows to obtain a better stationary solution.

Spalart [76] utilized a coordinate transform to approximate mean-flow non-parallelity across the computational domain. Following this idea, an
additional forcing term ($Z_c$) is introduced. We consider the following coordinate transformation from the Cartesian system $(x, y, z)$ to the non-Cartesian system $(\xi, \eta, \zeta)$

\[
\begin{pmatrix}
\frac{dx}{dt} \\
\frac{dy}{dt} \\
\frac{dz}{dt}
\end{pmatrix} = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
\Psi & 0 & \Omega
\end{pmatrix} \begin{pmatrix}
\frac{d\xi}{dt} \\
\frac{d\eta}{dt} \\
\frac{d\zeta}{dt}
\end{pmatrix} = J^{-1} \begin{pmatrix}
\frac{d\xi}{dt} \\
\frac{d\eta}{dt} \\
\frac{d\zeta}{dt}
\end{pmatrix},
\] (2.34)

where the Jacobian $J$ is given by

\[
J = \begin{pmatrix}
\frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} & \frac{\partial \xi}{\partial z} \\
\frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} & \frac{\partial \eta}{\partial z} \\
\frac{\partial \zeta}{\partial x} & \frac{\partial \zeta}{\partial y} & \frac{\partial \zeta}{\partial z}
\end{pmatrix} = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
-\Psi & 0 & \frac{1}{\Omega}
\end{pmatrix}.
\] (2.35)

We see that $x$ and $\xi$ are identical, as well as $y$ and $\eta$. The new wall-normal coordinate $\zeta$ is chosen so that the boundary-layer thickness and the viscous-sublayer thickness are independent of $x$ (or $\xi$) when expressed in terms of $\zeta$. $\Psi$ can be interpreted as the slope of the new coordinate lines with respect to the line $z = 0$. The meaning of $\zeta$ and $\Omega$ is not as clear, since they depend on a normalization, which eventually will be chosen so that, at the considered value of $x$, $\zeta$ and $z$ coincide, resulting in $\Omega = 1$. The basic Navier-Stokes equations can be written as follows in the original coordinate system $(x, y, z)$

\[
\frac{\partial \mathbf{U}}{\partial t} = \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \frac{\partial \mathbf{H}}{\partial z},
\] (2.36)

or in the transformed system $(\xi, \eta, \zeta)$

\[
\frac{\partial \mathbf{U}_1}{\partial t} = \frac{\partial \mathbf{F}_1}{\partial \xi} + \frac{\partial \mathbf{G}_1}{\partial \eta} + \frac{\partial \mathbf{H}_1}{\partial \zeta},
\] (2.37)

where

\[
\mathbf{U}_1 = \frac{1}{J} \mathbf{U}
\]

\[
\mathbf{F}_1 = \frac{1}{J} (\mathbf{F} \xi_x + \mathbf{G} \xi_y + \mathbf{H} \xi_z)
\]

\[
\mathbf{G}_1 = \frac{1}{J} (\mathbf{F} \eta_x + \mathbf{G} \eta_y + \mathbf{H} \eta_z)
\]

\[
\mathbf{H}_1 = \frac{1}{J} (\mathbf{F} \zeta_x + \mathbf{G} \zeta_y + \mathbf{H} \zeta_z).
\] (2.41)
2.4 Forcing terms

With \( J = |J| = \zeta_z \), one obtains

\[
\begin{align*}
U_1 & = \frac{1}{\zeta_z} U \\
F_1 & = \frac{1}{\zeta_z} F \\
G_1 & = \frac{1}{\zeta_z} G \\
H_1 & = \frac{\zeta_x}{\zeta_z} F + H.
\end{align*}
\]

Equation (2.37) can then be rewritten as

\[
\frac{\partial}{\partial t} \left( \frac{U}{\zeta_z} \right) = \frac{\partial}{\partial \xi} \left( \frac{F}{\zeta_z} \right) + \frac{\partial}{\partial \eta} \left( \frac{G}{\zeta_z} \right) + \frac{\partial}{\partial \zeta} \left( \frac{\zeta_x}{\zeta_z} F + H \right).
\]

As \( \zeta \) changes slowly in the streamwise direction, its \( x \)-derivative is formally written \( \zeta_x \), meaning that equations (2.25) or (2.26) are used for its computation. The same averaging method applies as for the forcing terms \( Z_0 \) and \( Z_1 \). We now identify \( \xi \) with \( x \) and \( \eta \) with \( y \), and set \( \Omega = 1 \) so that \( \partial / \partial \zeta \equiv \partial / \partial z \). It comes

\[
\frac{\partial U}{\partial t} = \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} + Z_c.
\]

As the analysis for \( Z_c \) applies to the non-parallelity of the mean flow, the mean flux \( \bar{F} \) is used. Further, as \( \Omega \equiv \partial z / \partial \zeta \) was set to 1, and because of the mathematical equality

\[
\Omega \zeta = \Psi \zeta
\]

(with \( \Psi = \partial z / \partial \xi \)), one finds that \( \Psi \zeta \) is zero and \( Z_c \) can be written as

\[
Z_c = \zeta_x \frac{\partial \bar{F}}{\partial z}.
\]

We adopt the definition of \( \zeta \) from Spalart [76], where the new coordinate is a weighted average of \( z^+ \) and \( z/\delta_0(X) \)

\[
\begin{align*}
\zeta(X, z) & = \zeta_0(X, z) + c(z) \\
\zeta_0(X, z) & = \left( z_2^P (10^{-3} z^+) + z_P (z/\delta_0(X)) \right) / (z_2^P + z_P).
\end{align*}
\]
The boundary-layer thickness at the considered spatial station $X$ is denoted as $\delta_0(X)$. The function $c(z)$ is used to make $\zeta$ and $z$ coincide at the considered $X$ station: its variation in $X$ is negligible. The mean flux $\overline{F}$ is

$$\overline{F} = \begin{bmatrix} -\bar{\rho}\bar{u} \\ -\bar{\rho}\bar{u}^2 - \bar{p} + \bar{\tau}_{xx} \\ -\bar{\rho}\bar{u}\bar{v} + \bar{\tau}_{xy} \\ -\bar{\rho}\bar{u}\bar{w} + \bar{\tau}_{xz} \\ -\overline{(u(E + p) - \bar{q}_x + \bar{u}\tau_{xx} + \bar{v}\tau_{xy} + \bar{w}\tau_{xz})} \end{bmatrix}$$

with

$$\bar{q}_x = -\frac{1}{(\gamma - 1)M_\infty^2 Pr Re} \frac{\bar{\mu}}{\zeta_x} \frac{\partial T}{\partial z}.$$  \hspace{1cm} (2.56)

The quantities with an overbar are the ones of the current time step averaged spatially in both wall-parallel directions.

### 2.5 Initial conditions

The different simulations are described in chapter 5. The cases $T_1$ and $T_2$ have the same Mach number ($M_\infty = 4.5$) but different wall temperatures, while the cases $M_30$, $M_45$ and $M_60$ have close-to-adiabatic wall temperatures at different free-stream Mach numbers.

For the cases $T_1$ and $M_45$, the final turbulent flow field from a separate transition simulation performed with a conventional TDNS method [3] is taken as initial condition. In the case $T_2$, the initial condition is the same as the one for $T_1$. At the beginning of the time integration at the very first spatial station, the wall temperature is ramped smoothly to its new level within a few time steps and the boundary layer is given some time to develop according to this new thermal boundary condition before marching the computational domain one step downstream. The initial conditions for
cases M30 and M60 are taken from case M45 by rescaling the flow field. At the very first spatial station, information about the spatial mean-flow development from previous marching steps is missing. Therefore, the forcing terms are approximated using a laminar compressible similarity solution for a zero-pressure gradient flat-plate boundary layer. This leads to a spatial transient during the first few spatial steps, which makes it difficult to reach statistical stationarity. Thus the solution has to be marched downstream after temporal transients have settled down appreciably even without having attained a stationary state.
Chapter 3
Numerical methods

3.1 Spatial discretization

Since the temporal DNS model requires periodic boundary conditions in the wall-parallel directions, a Fourier collocation scheme is used, employing a Fast Fourier Transform (FFT) algorithm. Because of the rapidity of the transform algorithm and its spectral accuracy this method is the most efficient one as long as the functions to be approximated are sufficiently smooth on a grid with a given resolution.

For the wall-normal direction, a finite-difference scheme with spectral-like properties is used. It was preferred to spectral methods using Chebyshev polynomials, which would have had the advantage of optimal accuracy, but would have unnecessarily limited the time-step with an explicit time-integration method [6]. The compact high-order Padé scheme applied here, obtained by defining an implicit left-hand side and explicit right-hand side stencil, achieves the highest possible formal accuracy compared to other one-parameter tridiagonal schemes [46].

The numerical solution employs a method-of-lines approach, whose first step is the spatial discretization. The continuous Navier-Stokes operator is not simply replaced by its discrete equivalent. For instance, the second derivatives appearing implicitly in the parabolic terms are split using the chain rule for stability reasons [1]. Furthermore, the diffusive and convective parts of the flux vectors are calculated one after another in order to use the computer storage capacity optimally.

3.1.1 Fourier collocation

The most natural choice in the case of periodic boundary conditions is to use Fourier trial functions. For the compressible Navier-Stokes equations,
the most efficient projection on Fourier space is done by collocation yielding a so-called pseudospectral scheme [11]. The coefficients of a finite Fourier expansion must be matched with the values of the function to be expanded at evenly spaced gridpoints. Highest efficiency is achieved by using FFT routines. Derivatives in the wall-parallel directions $x$ and $y$ are approximated by the derivative of the truncated Fourier series at the collocation points.

### 3.1.2 Compact finite-difference schemes

**Formulation**

The scheme used here is of sixth order accuracy at inner points, of fourth order at the next-to-boundary point and of third order at the boundary. Specific details, such as resolution properties, are given by Lele [45].

The approximation of the first and second derivatives for $\theta$ of a function $f(\theta) \in C^\sigma$ (where $\sigma \geq 1$) on an interval $\theta \in [0, 1]$ is given by

$$f^{(1)}_N = P^{(1)}_N(f_N) = M^{-1}_1 M_2 f_N$$

and

$$f^{(2)}_N = P^{(2)}_N(f_N) = N^{-1}_1 N_2 f_N$$

respectively. The vector of the values of $f(\theta)$ on the equidistant grid $\theta_N = \{\theta_0, \ldots, \theta_{N-1}\}$ is denoted $f_N$ while $f^{(1)}_N$ and $f^{(2)}_N$ represent the vectors of the corresponding first and second derivatives values. $P^{(1)}_N$ and $P^{(2)}_N$ are the first and second derivative discrete projection operators, which can be represented by the matrices $M^{-1}_1 M_2$ and $N^{-1}_1 N_2$. According to Lele [45], these quadratic matrices are defined as

$$M_1 = \begin{bmatrix}
2 & 4 \\
1 & 4 & 1 \\
1 & 3 & 1 \\
\vdots & \vdots & \vdots \\
1 & 3 & 1 \\
1 & 4 & 1 \\
4 & 2
\end{bmatrix},$$

(3.3)
where $h$ is the grid spacing in the basic interval. A discussion about the stability of the scheme can be found in Adams [1].
Mapping

As the resolution requirements in the wall-normal direction are not uniform, the gridpoints must be clustered in certain regions and can be rarer in others. Therefore, the evenly spaced grid in the computational variable $\theta \in [0, 1]$ is mapped onto $z \in [0, z_{\text{max}}]$ with $z_{\text{max}} = l_z$. The mapping function has to be continuously differentiable at least up to the order of the FD-approximation, otherwise the FD-schemes would exhibit a Gibbs-like phenomenon and their approximation order would be reduced. The following combined algebraic/analytic mapping function is used

$$\theta_j = \frac{j}{N_z - 1} \quad \text{with} \quad j = 0, \ldots, N_z - 1$$

(3.7)

$$z_j = \frac{z_{\text{max}} z_{1/2} \Phi_j}{(z_{\text{max}} - z_{1/2}) + (2z_{1/2} - z_{\text{max}}) \Phi_j}$$

(3.8)

where $z_{1/2}$ is the image of $\theta_j = 1/2$. The metric coefficients for the first and second derivatives are given by

$$m_j^{(1)} = \frac{(z_{\text{max}} - z_{1/2})^2 + (2z_{1/2} - z_{\text{max}}) \Phi_j^2}{z_{\text{max}} z_{1/2} (z_{\text{max}} - z_{1/2}) \left( a + \frac{a_1}{a_3} \cosh \left( \frac{\theta_j - a_2}{a_3} \right) \right)}$$

(3.9)

$$m_j^{(2)} = \frac{\Sigma_1}{\Sigma_2} - \frac{\Sigma_3}{\Sigma_4}$$

(3.10)

where

$$\Phi_j = a \theta_j + b + a_1 \sinh \left( \frac{\theta_j - a_2}{a_3} \right)$$

$$\Sigma_1 = 2 (2z_{1/2} - z_{\text{max}}) (z_{\text{max}} - z_{1/2}) + (2z_{1/2} - z_{\text{max}}) \Phi_j$$

$$\Sigma_2 = z_{\text{max}} z_{1/2} (z_{\text{max}} - z_{1/2})$$

$$\Sigma_3 = (z_{\text{max}} - z_{1/2})^2 + (2z_{1/2} - z_{\text{max}}) \Phi_j^2 a_1^2 a_3 \sinh \left( \frac{\theta_j - a_2}{a_3} \right)$$

$$\Sigma_4 = z_{\text{max}} z_{1/2} (z_{\text{max}} - z_{1/2}) \left( a + \frac{a_1}{a_3} \cosh \left( \frac{\theta_j - a_2}{a_3} \right) \right)^2$$

$$a = 1 - a_1 \left( \sinh \left( \frac{1 - a_2}{a_3} \right) + \sinh \left( \frac{a_2}{a_3} \right) \right)$$

$$b = a_1 \sinh \left( \frac{a_2}{a_3} \right).$$
The mappings are tuned by choosing a suitable set of parameters $z_{\text{max}}$, $z_{1/2}$, $a_1$, $a_3$ and $z_{mv}$. The parameter $a_2$ is calculated using the condition that $z_{mv}$ coincides with the image of the inflection point of the function $\sinh((\theta-a_2)/a_3)$. Therefore, the following transcendental equation is solved for $a_2$

$$z_{mv} - z(a_2) = 0$$

(3.11)

where $z(a_2)$ is calculated according to the continuous form of equation (3.8) with variable $a_2$ and $\theta = a_2$. The derivatives with respect to $z$ are computed from the derivatives with respect to $\theta$ with

$$\frac{\partial f}{\partial z} = m^{(1)} \frac{\partial f}{\partial \theta}$$

(3.12)

$$\frac{\partial^2 f}{\partial z^2} = m^{(1)^2} \frac{\partial^2 f}{\partial \theta^2} + m^{(2)} \frac{\partial f}{\partial \theta}.$$ 

(3.13)

The mapping-parameter sets used for the different simulations (defined in chapter 5) are given in table 3.1.

<table>
<thead>
<tr>
<th>Case</th>
<th>T1</th>
<th>T2</th>
<th>M30</th>
<th>M45</th>
<th>M60</th>
</tr>
</thead>
<tbody>
<tr>
<td>$z_{\text{max}}$</td>
<td>15</td>
<td>15</td>
<td>15</td>
<td>15</td>
<td>25</td>
</tr>
<tr>
<td>$z_{1/2}$</td>
<td>3.5</td>
<td>0.6</td>
<td>2.5</td>
<td>3.4</td>
<td>5.0</td>
</tr>
<tr>
<td>$z_{mv}$</td>
<td>1.5</td>
<td>8.0</td>
<td>1.0</td>
<td>1.55</td>
<td>2.0</td>
</tr>
<tr>
<td>$a_1$</td>
<td>0.7</td>
<td>0.55</td>
<td>0.7</td>
<td>0.7</td>
<td>0.7</td>
</tr>
<tr>
<td>$a_3$</td>
<td>0.8</td>
<td>0.45</td>
<td>0.8</td>
<td>0.7</td>
<td>0.8</td>
</tr>
</tbody>
</table>

**Filtering**

Aliasing errors result from the generation of scales with wavelengths smaller than twice the grid spacing in a considered direction. Responsible for that are the nonlinear terms in the Navier-Stokes equations, in which the three coordinate directions are coupled, so that aliasing errors can transfer across the dimensions and solution components. The wall-normal coordinate is particularly sensitive to that problem, as the resolution requirements are
not homogeneous in this direction. This is partially accounted for by the coordinate mapping in $z$. Nevertheless, aliasing errors can still occasionally become troublesome, so that a low-pass compact filter is applied every third to fifth time step in the wall-normal direction to cope with them. It is of sixth order formal accuracy at the inner points and of fourth order at the three near-boundary nodes [45]. At all nodes the waves with a normalized wave number of $\pi$ are filtered exactly to zero. The filter has the following form at the inner gridpoints

$$ \beta \hat{f}_{i-2} + \alpha \hat{f}_{i-1} + \hat{f}_i + \alpha \hat{f}_{i+1} + \beta \hat{f}_{i+2} = $$

$$ a f_i + \frac{d}{2} (f_{i+3} + f_{i-3}) + \frac{c}{2} (f_{i+2} + f_{i-2}) + \frac{b}{2} (f_{i+1} + f_{i-1}) \quad (3.14) $$

where $\hat{f}_i$ represents the filtered value of $f$ at the node $i$. Here we use

$$ \alpha = 0.625 \quad \beta = \frac{3 - 2\alpha}{10} $$

$$ a = \frac{2 + 3\alpha}{4} \quad b = \frac{6 + 7\alpha}{8} \quad c = \frac{6 + \alpha}{20} \quad d = \frac{2 - 3\alpha}{40} $$

The explicit fourth-order near-boundary schemes are

$$ \hat{f}_1 = \frac{15}{16} f_1 + \frac{1}{16} (4f_2 - 6f_3 + 4f_4 - f_5) $$

$$ \hat{f}_2 = \frac{3}{4} f_2 + \frac{1}{16} (f_1 + 6f_3 - 4f_4 + f_5) $$

$$ \hat{f}_3 = \frac{5}{8} f_3 + \frac{1}{16} (-f_1 + 4f_2 + 4f_4 - f_5) $$

$$ \hat{f}_N = \frac{15}{16} f_N + \frac{1}{16} (4f_{N-1} - 6f_{N-2} + 4f_{N-3} - f_{N-4}) $$

$$ \hat{f}_{N-1} = \frac{3}{4} f_{N-1} + \frac{1}{16} (f_N + 6f_{N-2} - 4f_{N-3} + f_{N-4}) $$

$$ \hat{f}_{N-2} = \frac{5}{8} f_{N-2} + \frac{1}{16} (-f_N + 4f_{N-1} + 4f_{N-3} - f_{N-4}). $$

### 3.2 Time advancement

With a method-of-lines formulation, it is possible to get a clearly structured code as the spatial discretization is fully decoupled from the time integration. The system of partial differential equations (PDE) is first transformed
into a system of ordinary differential equations (ODE) by applying the spatial discretization methods, thus yielding the temporal derivative of the solution vector.

The explicit Runge-Kutta schemes are of particular interest, as they are robust and mathematically convenient to handle for stability analysis [1]. Experience shows that for Runge-Kutta schemes of third to fourth order the accuracy requirements and stability restrictions demand approximately the same time-step limitations at moderate to high Mach numbers (when a finite-difference discretization is used in the wall-normal direction) [1].

3.2.1 Explicit Runge-Kutta scheme

In conventional notation the third-order explicit Runge-Kutta scheme used in this work for the time integration is written as

\[
\begin{align*}
    k_1 &= \tau \cdot F(t_n, U_n) \\
    k_2 &= \tau \cdot F(t_n + \frac{2}{3} \tau, U_n + \frac{2}{3} k_1) \\
    k_3 &= \tau \cdot F(t_n + \frac{2}{3} \tau, U_n + \frac{1}{4} k_1 + \frac{5}{12} k_2) \\
    U_{n+1} &= U_n + \frac{1}{4} k_1 + \frac{3}{20} k_2 + \frac{3}{5} k_3
\end{align*}
\]

(3.16)

where \( \tau \) is the time-step size and \( F \) represents the right-hand side of the Navier-Stokes equations, i.e. the time derivative of \( U \). A low-storage version of this scheme [86] is used here which occupies only two additional storage units per variable and gridpoint. If \( W \) and \( T \) are the storage units and the last time-step’s solution is stored in \( Q \), then the algorithm can be written as

\[
\begin{align*}
    T &\leftarrow F(t, Q) \\
    Q &\leftarrow Q + \frac{1}{4} \tau T \\
    W &\leftarrow Q + \left( \frac{2}{3} - \frac{1}{4} \right) \tau T \\
    T &\leftarrow F(t + \frac{2}{3} \tau, W) \\
    Q &\leftarrow Q + \frac{3}{20} \tau T \\
    W &\leftarrow Q + \left( \frac{5}{12} - \frac{3}{20} \right) \tau T \\
    T &\leftarrow F(t + \left( \frac{1}{4} + \frac{5}{12} \right) \tau, W) \\
    Q &\leftarrow Q + \frac{3}{5} \tau T
\end{align*}
\]
3.2 Time advancement

3.2.2 Time-step size

A necessary condition for a stable time integration is that the eigenvalues of the spatially discretized Navier-Stokes equations belong to the stability domain of the considered Runge-Kutta scheme. This is secured by a dynamic time-step control. We consider a scalar model advection-diffusion equation

\[
\frac{\partial \phi}{\partial t} + a_1 \frac{\partial \phi}{\partial x} + a_2 \frac{\partial \phi}{\partial y} + a_3 \frac{\partial \phi}{\partial z} = d \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} \right). \tag{3.17}
\]

If \( \hat{\phi} \) is the Fourier transform of \( \phi(x, y, z) \), equation (3.17) can be rewritten in the spectral space

\[
\frac{\partial \hat{\phi}}{\partial t} + i(a_1 \alpha + a_2 \beta + a_3 \gamma) \hat{\phi} + d(a^2 + \beta^2 + \gamma^2) \hat{\phi} = 0 \tag{3.18}
\]

where \( \alpha, \beta \) and \( \gamma \) are the dual variables of \( x, y \) and \( z \). The preceding equation is equivalent to

\[
\frac{\partial \hat{\phi}}{\partial t} = A \hat{\phi} \tag{3.19}
\]

with \( A = -i(a_1 \alpha + a_2 \beta + a_3 \gamma) - d(a^2 + \beta^2 + \gamma^2) \).

The discrete Fourier transform is now considered with \( N_x \times N_y \times N_z \) points in the \( x, y \) and \( z \) directions. Since we are only interested in an approximation which is valid locally, the assumption of periodicity in the \( z \)-direction is reasonable. The discrete wave numbers are approximated as follows

\[
|\alpha| \leq \frac{\pi}{\Delta_x} , \quad |\beta| \leq \frac{\pi}{\Delta_y} , \quad |\gamma| \leq \frac{\pi}{\min(\Delta_z)} ,
\]

where \( \Delta_x, \Delta_y \) and \( \Delta_z \) are the grid spacings in the corresponding directions. Note that in the wall-normal direction \( z \) a non-evenly spaced grid is admitted. The constants \( a_1, a_2 \) and \( a_3 \) are estimated from the maximum eigenvalues of the hyperbolic part of the Navier-Stokes equations and the constant \( d \) from the maximum of the parabolic part

\[
\begin{align*}
|a_1| & \leq |u| + c \\
|a_2| & \leq |v| + c \\
|a_3| & \leq |w| + c \\
d & \leq d_{\text{max}} = \max \left( \frac{1}{\mu} \frac{\rho}{Re}, \frac{1}{(\gamma-1)} M_{\infty}^2 P r \rho Re \right)
\end{align*}
\]
where

\[ c = \sqrt{T} / M_\infty \]  \hspace{1cm} (3.20)

represents the local value of the speed of sound. The factor \(1/\rho \) in \( d_{\max} \) comes from scaling considerations. From a CFL-like condition given by the restriction of the resulting stability function to its stability domain, follows the time-step limitation

\[ \tau \leq \frac{CFL}{A_{\max}} \]  \hspace{1cm} (3.21)

where

\[ A_{\max} = \pi \max \left( \frac{|u| + \sqrt{T}}{\Delta_x} + \frac{|v| + \sqrt{T}}{\Delta_y} + \frac{|w| + \sqrt{T}}{\Delta_z} + \pi d_{\max} \left( \frac{1}{\Delta_x^2} + \frac{1}{\Delta_y^2} + \frac{1}{\Delta_z^2} \right) \right) \]  \hspace{1cm} (3.22)

As this CFL number is formulated in the spectral space it is larger than the corresponding real-space CFL-number by a factor of \( \pi \) for the convective limit and by a factor of \( \pi^2 \) for the viscous limit.

### 3.3 Filtering of the oddball modes

For consistency during time-integration with the real Fourier expansions used in the periodic directions, the following filtering operation is performed. Its necessity is demonstrated by means of the linear convection equation

\[ \frac{\partial u}{\partial t} + C \frac{\partial u}{\partial x} = 0 \]  \hspace{1cm} (3.23)

where \( u \) is real and \( C \) is a real constant. The dual equation of (3.23) after a discrete Fourier transform of length \( N \) \((N \text{ even})\) is

\[ \sum_{k=-N/2+1}^{N/2} \frac{\partial \hat{u}_k}{\partial t} e^{ikx} + C \sum_{k=-N/2+1}^{N/2} ik \hat{u}_k e^{ikx} = 0 \]  \hspace{1cm} (3.24)

where the \( \hat{u}_k \) are the complex coefficients of the Fourier series of \( u \). In a Fourier transform of length \( N \) the wave number \( k = N/2 \) is commonly
3.3 Filtering of the oddball modes

referred to as oddball wavenumber. This oddball mode, as well as the 0-mode, has real Fourier coefficients, i.e. \( \text{Im}(\hat{u}_0) = \text{Im}(\hat{u}_{N/2}) = 0 \) [15]. Equation (3.24) requires for the modes 0 and \( N/2 \) that

\[
\frac{\partial \hat{u}_0}{\partial t} e^{i \frac{N}{2} x} = -Ci0 \hat{u}_0 e^{i \frac{N}{2} x} \tag{3.25}
\]

\[
\frac{\partial \hat{u}_{N/2}}{\partial t} e^{i \frac{N}{2} x} = -C \frac{N}{2} \hat{u}_{N/2} e^{i \frac{N}{2} x} \tag{3.26}
\]

The 0-mode causes no problem but the oddball mode must be considered more carefully. The left-hand side of equation (3.26) is real, and consistency with the right-hand side requires that \( \hat{u}_{N/2} = 0 \). It is thus necessary to explicitly zero out the oddball component during the computation. As the time integration is performed in real space it is desirable to use an efficient filtering method with a real-space formulation. The method proposed by Sandham & Reynolds [66] is chosen. The real-space variable at the grid-point with indices \((j_1, j_2)\) in a wall-parallel plane is denoted \( V_{j_1, j_2} \). The corresponding filtered variable \( V^F_{j_1, j_2} \) is computed after every time step (including the intermediate Runge-Kutta steps) for every component of the solution vector \( U \) by applying the following summation formula

\[
V^F_{j_1, j_2} = V_{j_1, j_2} + (-1)^{j_2+1} \frac{1}{N_y} \sum_{\nu_2=0}^{N_y-1} (-1)^{\nu_2} V_{j_1, \nu_2}
\]

\[
+ (-1)^{j_1+1} \frac{1}{N_x} \sum_{\nu_1=0}^{N_x-1} (-1)^{\nu_1} V_{\nu_1, j_2}
\]

\[
+ (-1)^{j_1+j_2} \frac{1}{N_x N_y} \sum_{\nu_1=0}^{N_x-1} \sum_{\nu_2=0}^{N_y-1} (-1)^{\nu_1+\nu_2} V_{\nu_1, \nu_2} \tag{3.27}
\]

where \( j_1 = 0, \ldots, N_x - 1 \) and \( j_2 = 0, \ldots, N_y - 1 \). This method was found to be substantially cheaper than the alternative method of Fourier transforming, zeroing the oddball and inverse transforming.
Chapter 4

Code parallelization

The original code was developed and optimized to run on a vector computer [29]. When the decision of parallelizing the code was taken, it was accompanied by the following constraints. First, the parallel platform was to be the CRAY T3D located at the EPFL (Ecole Polytechnique Fédérale in Lausanne). Second, the general structure of the code, as well as the structure of the input and output files should remain essentially unchanged. It is easy to understand the second reason, as changing the structure of a code whose length is several thousands of lines would be equivalent to writing a new code, which was not the aim of the work. However, the given structure is far from optimal for a massively parallel machine as it implies numerous data passing phases. They could probably have been minimized by rewriting the code, thus increasing greatly its general performance.

The portability of a code is usually desirable: with no or few adaptations, the code can run on different machines. It also means that a portable code is written so that it is suitable for various architectures after modest changes. This implies that the code will be suboptimal for certain platforms. In the present case, a compromise was chosen between portability and performance optimization. Although a CRAY-specific message passing language is used, minor modifications would allow to port the parallelized version of the code to other parallel architectures.

A code can be parallelized automatically or manually. In the former case, the parallelization work of the compiler can be influenced by directives inserted in the program. The manual parallelization implies that the programmer organizes the data and work distribution as well as the communications between the processors by writing the necessary commands within the program. The first method allows to quickly have a parallelized code but gives only few insights in the way the parallelization was performed: the code behaves somehow like a black box. The second method undoubtedly takes
4.1 The CRAY T3D of the EPFL

The EPFL has acquired in 1994 a CRAY T3D MC256-8 massively parallel computer. It is equipped with 256 DEC Alpha EV4 microprocessors (DEC chip 21064), each with 64 Mbytes of local DRAM and a peak performance of 150 MFLOPS. The DEC Alpha is a reduced instruction set computing (RISC) processor, which is cache based, has pipelined functional units, issues two instructions per cycle and supports IEEE standard 64-bit floating-point arithmetic. Each processing element (PE) in the T3D system comprises the DEC Alpha microprocessor, a local memory and the support logic. The PE is the basic computational unit in the T3D system’s multiple instruction multiple data (MIMD) architecture. A T3D system node consists of two PEs sharing the switch and network support logic, as illustrated in figure 4.1. The PEs are connected by a very fast bidirectional

![T3D compute node and three-dimensional torus network](image)

Figure 4.1: T3D compute node (left) and three-dimensional torus network (right).
three-dimensional torus system interconnect network, which allows for a peak interprocessor communication rate of 300 Mbytes per second in every direction. The performance of the system interconnect is augmented by latency hiding mechanisms (pre-fetch queue and read-ahead mode for a few data words, block transfer engine for larger data sets).

The memory in the T3D is physically distributed among processors, but is globally addressable (any microprocessor can address any memory location in the system).

### 4.2 Basic parallelization

In order to minimize the communications between the PEs, the data must be distributed so that they remain *as local as possible*. This means that the data needed by a processor should be in its local memory and not in the one of a remote PE. We have to consider mainly two categories of operations on large data arrays. The fast Fourier transforms (FFT) and plane-averaging operations require wall-parallel data vectors. As for the compact finite-difference schemes (derivation and filtering in $z$), they are applied on data vectors normal to the wall. The resulting two possible data distributions are illustrated in figure 4.2. In both cases, the computational domain is divided into "slices" of equal thickness in such a way that each PE receives exactly one data slice, which is stored in its local memory. Doing so, the load balancing is optimal. Throughout the execution of the program, and depending on which operation has to be performed, data are switched from one distribution to the other. As the operations in the homogeneous

![Diagram of horizontal and vertical data distribution on 4 PEs.](image)

*Figure 4.2: Horizontal (left) and vertical (right) data distribution on 4 PEs.*
4.2 Basic parallelization

Wall-parallel directions \( x \) and \( y \) are more numerous than in the wall-normal direction, the reference data distribution is the one with horizontal slices. Data are switched into the other distribution (vertical slices) only to perform operations in \( z \), and moved back immediately after completion.

It was mentioned earlier that the parallel code should be "tuned" to the T3D architecture as much as possible, without going too far and making the code no longer portable. In the light of this reflection, the SHMEM programming method was chosen for the message-passing. The CRAY specific shared memory (SHMEM) programming method allows low-level explicit data communication without synchronization. This method makes the programmer responsible for managing data transfers and communications by explicitly specifying a local address and a remote address between which data transfer has to take place. Two basic routines are used: \texttt{SHMEM\_GET} (transfers data from the remote address to the local address) and \texttt{SHMEM\_PUT} (transfers data from the local address to the remote address). The change from one data distribution to the other happens as follows. Each PE is responsible for writing its local data (with \texttt{SHMEM\_PUT}, see figure 4.3) on the corresponding PE in the new distribution. This is performed independently, but the operations with the new distribution only begin after a synchronization point which ensures that all the data have been transfered.

![Diagram](image_url)

*Figure 4.3: Data array initially distributed vertically on 4 PEs (left) is then redistributed horizontally (right). In the middle is illustrated the array part that PE 3 must write on the other PEs for the new distribution.*
The data distribution adopted here does not require the use of parallel FFT. The computational domain is divided in such a way that each PE can work independently on its local data with the usual FFT routines. To achieve better performances, optimized CRAY FFT routines were implemented in the code.

In order to make the code portable, it would basically be sufficient to replace the CRAY FFT routines and the SHMEM commands (SHMEM_GET, SHMEM_PUT, ...) by appropriate ones for the new platform.

As parallel input/output capabilities were not implemented on the T3D in Lausanne, the I/O task was given to the MASTER processor (i.e. the PE whose number is 0). Beside having its share of work like all other PEs, the MASTER is also responsible, at the beginning of a run, for reading initial data which it copies on the other PEs, and for reading the initial flow field which it distributes on the other PEs. At the end of a run, it writes the final data and the complete flow field to a file.

The parallelization method described above allows to optimize the code performances on the T3D but also leads to certain restrictions. The 256 processors of the T3D are allocated to the users in partitions, each containing a number of PEs which is a power of 2. One could of course, for the sake of flexibility, use fewer PEs than the allocated number, but this would be a waste of resources: one always tries to use all the allocated PEs and further more to use them in parallel, avoiding serial regions (i.e. regions where some processors do not work). For the distributed directions $y$ and $z$ (i.e. directions along which the computational domain is cut in “slices”), the total number of points $l$ must be an integer multiple of the number of PEs, so that the data slices can have equal dimensions. Also, since a slice must contain at least one “layer” of data points, the number of PEs must be less than the smallest number of points of the distributed directions. This means that for a given simulation grid, the maximum number of PEs is given by the above-mentioned condition while the minimum number is a function of the size of the computational domain, which must find enough place in the total memory of the allocated PEs.

A further constraint exists for the number of gridpoints in the wall-parallel directions $x$ and $y$. The FFT routines used here can perform the transform

---

$1$ in the directions $x$ and $y$ where the real to half-complex FFT are performed, the number of gridpoints in one direction is $n$ (i.e. length of the transform), while the total number of points in the same direction is $np = n + 2$. The two additional points are needed to store the complex coefficients of the transformed vector.
of vectors with any even length $n$. However, the number of operations required for this is minimal when $n$ is a power of 2, in which case the number of floating-point operations is approximately $\frac{5}{2} n \log_2 n$. If $n$ contains factors of 3, performance is slightly worse. If $n$ contains powers of 5, it is still slightly worse. Worst performance is when $n$ is twice a prime number, in which case the number of operations is approximately $4n^2$. Thus, particular attention must be paid to the prime factorization of $n$ in the wall-parallel directions so that the FFT remain "fast".

The spanwise direction $y$ is affected by both the above-mentioned constraints. A compromise between flexibility and optimal resource utilization was made for this direction by implementing "ghost cells". It allows to consider separately the constraints on the total number of points and the number of gridpoints, which are no longer linked by the equation $np = n+2$.

### 4.3 Optimization

The CRAY T3D is a computer system built around a commodity microprocessor, whose interconnect between the PEs is extremely efficient in terms of bandwidth and latency. As such, most optimization effort is applied to the single PE code.

The Alpha EV4 processor runs at 150 MHz and is capable of 150 MFLOPS of peak performance. The bandwidth from the primary cache is one 64-bit word per clock (1.2 Gbytes/sec). The peak bandwidth from the main memory is approximately one word per 4 clock periods (320 Mbytes/sec). Combining those two figures with the small 1024 word data cache of the EV4, it becomes clear that most single PE optimization centers on efficient memory and cache utilization.

After the basic parallelization was completed, following measures were applied to enhance the code performance:

- **loop unrolling**:
  Unrolling inner loops allows to use the data in the cache more efficiently and to better utilize functional unit pipelining (for multiplication and addition). In the example below ($a$ : basic loop, $b$ : unrolled loop with stride 3), the three values of the arrays in case $b$) are loaded in the cache so that they are brought faster to the registers and the pipelined functional units can be used.
4 Code parallelization

a) real a(m), b(m)

\[
\text{do } i = 1, m \\
a(i) = a(i) + 2.0*b(i) \\
\text{enddo}
\]

b) real a(m), b(m)

\[
\text{do } i = 1, m, 3 \\
a(i) = a(i) + 2.0*b(i) \\
a(i+1) = a(i+1) + 2.0*b(i+1) \\
a(i+2) = a(i+2) + 2.0*b(i+2) \\
\text{enddo}
\]

- **scalar replacement**:
  In a loop, when an element of an array is referenced which remains constant in this loop, it is then advantageous to use a temporary scalar instead. The latter can be kept in a register, resulting in fewer memory references. In the example below, the constant array element of the inner loop c(j) in a) has been replaced by a scalar in b).

a) real a(m,n), b(n)

\[
\text{do } j = 1, n \\
\text{do } i = 1, m \\
a(i,j) = a(i,j) + 3.0*b(j) \\
\text{enddo} \\
\text{enddo}
\]

b) real a(m,n), b(n)

\[
\text{do } j = 1, n \\
\text{const } = b(j) \\
\text{do } i = 1, m \\
a(i,j) = a(i,j) + 3.0*const \\
\text{enddo} \\
\text{enddo}
\]

- **divide operation**:
  The divide operation is expensive and the divide unit is not pipelined. When all the elements of an array must be divided by a constant, a much higher efficiency is reached by multiplying the array by the reciprocal of the constant, which is calculated once before the loop.

- **memory writes**:
  The EV4 chip has 4 write buffers. As soon as a write buffer contains a valid entry, it initiates a buffer flush sequence. While this sequence completes, other stores can issue and continue to fill the write buffer. If all four write buffers contain a valid entry, the store queue shuts down and further store instructions have to wait for a free entry. Thus, in order to have the largest possible bandwidth, it is better to avoid 4 or more store streams in an inner loop. Going from 3 to 4 streams makes the bandwidth drop by a factor of 4.
• *synchronization*:
  During the basic parallelization, it is comfortable to incorporate many synchronization points (BARRIER) in order to have a tight control on the temporal progress of operations on all PEs. Once the parallel code works, it is usually possible to remove some of those synchronization points.

• *read-ahead mode*:
  By switching on this address mode, data for the next cache line are automatically brought into the read-ahead buffer. If the next load which generates a miss is sequential, then the four next words will already be in the read-ahead buffer, saving many additional clock periods. With the read-ahead mode enabled an element of a cache line can be loaded into a register every 15 clock periods (instead of 25 if the mode is disabled).

### 4.4 Performances

The performance of the optimized code was measured with the CRAY performance monitoring tool MPP Apprentice. The test was carried out on the computation grid used for the simulations. It has a total of 326 points in the streamwise direction, 192 in the spanwise direction and in the direction normal to the wall, distributed on 64 PEs. The effective length of the transform is 324, 180 (the rest are ghost cells) and 190, respectively. The measured average performance on 64 PEs is 780 MFLOPS, or 12 MFLOPS/PE. The best measurable procedure reaches 21 MFLOPS/PE while CRAY subroutines (like FFT routines) run typically at 25 MFLOPS/PE. The code needs 8.3 µsec of wall-clock time to compute one time-step for one gridpoint. For comparison, the procedures of the NAS (Numerical Aerospace Simulation Facility) Kernel benchmark reach between 18 and 63 MFLOPS/PE on one PE when highly optimized for the T3D architecture, while a matrix multiply procedure from an optimized library (MXM) achieves 107 MFLOPS/PE. In contrast to these short and highly tuned procedures, a code solving compressible turbomachinery flows and using a portable message-passing language (PVM) reached an averaged performance of 8 MFLOPS/PE on 16 PEs after optimization [35].

The performance analysis reveals that 16% of the elapsed time is spent on executing “work” instructions (additions, multiplications, divisions). In
spite of the optimization effort, loading instruction and data caches takes 30.6% of the elapsed time, confirming the weak point of the EV4 chip. Waiting on shared memory operations (like data transfer with SHMEM.GET and SHMEM.PUT, the BARRIER synchronization points, the MASTER serial regions) necessitates 16.8% of the time. Although the files that are read at the beginning of a run and written at the end are quite large (ca. 475 Mbytes), the percentage of time spent in I/O operations is only of 0.04%. Finally, the intrinsic functions (so-called “uninstrumented” routines: routines in which the performance tool can not count the operations) take 35.6% of the time, where 34.4% is for the CRAY FFT routines and 1.2% for other intrinsic functions.

4.5 Scalability

The scalability of the code was assessed on a grid with $50 \times 32 \times 128$ points distributed on 8, 16 and 32 PEs. For the reasons mentioned above, the computational domain could not be distributed on fewer than 8 or more than 32 PEs. Figure 4.4 represents the elapsed time needed to perform 100 time steps on different partitions. The scalability is excellent, as the required time drops roughly by a factor of 2 when the number of PEs is doubled. This is a sign that the workload is very well balanced among the processors (as was explicitly required by the chosen parallelization method) and that the network contention is not a problem.

![Figure 4.4: Scalability of the parallelized code.](image-url)
Chapter 5

Simulation parameters and results

Two sets of data are presented in the following. The first one comprises two cases with the same free-stream Mach number but with different wall temperatures. In the second set, three cases have an isothermal wall with a close-to-adiabatic temperature at different free-stream Mach numbers. The

<table>
<thead>
<tr>
<th>Table 5.1: Main simulation parameters.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case</td>
</tr>
<tr>
<td>M∞</td>
</tr>
<tr>
<td>u∞ [m/s]</td>
</tr>
<tr>
<td>p∞ [Pa]</td>
</tr>
<tr>
<td>T∞ [K]</td>
</tr>
<tr>
<td>μ∞ [kg/(m \cdot s)]</td>
</tr>
<tr>
<td>R* [J/(kg \cdot K)]</td>
</tr>
<tr>
<td>γ</td>
</tr>
<tr>
<td>Re</td>
</tr>
<tr>
<td>Pr</td>
</tr>
<tr>
<td>CFL</td>
</tr>
<tr>
<td>T_w/T∞</td>
</tr>
<tr>
<td>l_x/δ_{1,io,m}</td>
</tr>
<tr>
<td>l_y/δ_{1,io,m}</td>
</tr>
<tr>
<td>l_z/δ_{1,io,m}</td>
</tr>
<tr>
<td>N_x</td>
</tr>
<tr>
<td>N_y</td>
</tr>
<tr>
<td>N_z</td>
</tr>
</tbody>
</table>
two sets are first presented separately (chapter 6 and 7), then some issues common to both sets are discussed in chapter 8. The main parameters for all our simulations are found in table 5.1. The data are non-dimensionalized with the reference values given in section 2.2. Unless mentioned otherwise, the lengths are normalized with the compressible thickness $\delta_c$ of the corresponding mean flow, see equation (2.11). The relevant integral values and other important figures of the simulations are summarized in table 5.2. Contrary to the values in table 5.1, which are set at the beginning of a simulation and remain constant, the ones listed here are simulation results and can not be enforced (except $t_s$ and $n_s$). The different $Re_\theta$ (based on momentum thickness and free-stream viscosity) are all between 3000 and 4000, while the $Re_{\delta_2}$ (based on the wall viscosity) span a larger range (500...3500). The size of the computational domains, expressed in wall units, is rather at

<table>
<thead>
<tr>
<th>Case</th>
<th>T1</th>
<th>T2</th>
<th>M30</th>
<th>M45</th>
<th>M60</th>
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<tr>
<td>$Re_{\delta_1}$</td>
<td>37269</td>
<td>30733</td>
<td>17749</td>
<td>29463</td>
<td>50643</td>
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<tr>
<td>$Re_{\delta_2}$</td>
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<td>3569</td>
<td>1174</td>
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<td>500</td>
</tr>
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<td>$Re_\theta$</td>
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<td>3953</td>
<td>3028</td>
<td>3305</td>
<td>2945</td>
</tr>
<tr>
<td>$H_{12}$</td>
<td>9.825</td>
<td>7.775</td>
<td>5.861</td>
<td>8.914</td>
<td>17</td>
</tr>
<tr>
<td>$C_f \cdot 10^3$</td>
<td>1.538</td>
<td>1.455</td>
<td>2.016</td>
<td>1.514</td>
<td>1.142</td>
</tr>
<tr>
<td>$u_\tau \cdot 10^2$</td>
<td>5.688</td>
<td>2.800</td>
<td>4.978</td>
<td>5.617</td>
<td>6.140</td>
</tr>
<tr>
<td>$Re \cdot u_\tau / \nu_w$</td>
<td>33</td>
<td>235</td>
<td>78</td>
<td>32</td>
<td>16</td>
</tr>
<tr>
<td>$\delta_{0^+}^+$</td>
<td>250</td>
<td>1621</td>
<td>372</td>
<td>220</td>
<td>133</td>
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<tr>
<td>$l_x^+$</td>
<td>487</td>
<td>3510</td>
<td>549</td>
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<td>395</td>
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<tr>
<td>$\Delta_x^+$</td>
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<td>2.9</td>
<td>2.9</td>
<td>1.3</td>
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<td>12</td>
<td>9</td>
<td>26</td>
<td>26</td>
</tr>
<tr>
<td>$n_s$</td>
<td>40</td>
<td>40</td>
<td>43</td>
<td>81</td>
<td>40</td>
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</table>
the lower limit for the streamwise and spanwise directions. The cold-wall case T2 and case M45, with a significantly enlarged computational domain, are less concerned by that remark. Clearly, the limited amount of available CPU time and computational memory constrains the choice of the domain size. However, the assumption of local parallelism of the mean-flow, essential for the ETDNS method, requires a relatively short streamwise extent for the computational domain. Further, all our domain sizes well exceed the dimensions (in wall units) of the minimal channel simulations of Jimenez & Moin [36] which are about 300 and 100 wall units in the streamwise and spanwise directions, respectively. Jimenez & Moin found that for these minimum dimensions, second-order statistics were still in excellent agreement with experimental data below \( z^+ \approx 40 \), although two-point correlations over distances of half the domain size were rather large.

As mentioned in section 2.5, the cases M45 and T1 share the same flow field as initial condition for the simulation. Besides, they have many common parameters (\( M_\infty, Pr, T_w, u_*^*, T_*^* \), ...). However, other elements make that the results for those two cases show some differences. First, the original flow field is adapted to two different domain sizes with different resolutions. Then the time integration history also differs. This finally re-

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**Table 5.3: Parameters of other simulations: incompressible boundary layer (Spalart), compressible boundary layer (Guarini et al.), incompressible channel flow (Moser et al.).** Spalart uses spectral schemes in the three spatial directions and employs the \( \frac{2}{3} \)-rule for de-aliasing, so that the number of usable spectral modes is \( \frac{2}{3} \) the number of gridpoints for each direction.

<table>
<thead>
<tr>
<th>Authors</th>
<th>Spalart [76]</th>
<th>Guarini et al. [28]</th>
<th>Moser et al. [54]</th>
</tr>
</thead>
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<tr>
<td>( M_\infty )</td>
<td>0</td>
<td>0</td>
<td>2.5</td>
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<td>( Re_\theta )</td>
<td>670</td>
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</tr>
<tr>
<td>( l_x^+ )</td>
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<td>2271</td>
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<tr>
<td>( l_y^+ )</td>
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<td>2850</td>
<td>1135</td>
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</tr>
<tr>
<td>( \Delta_y^+ )</td>
<td>9.6</td>
<td>13.4</td>
<td>5.2</td>
</tr>
<tr>
<td>( N_x )</td>
<td>256 (( \cdot \frac{2}{3} ))</td>
<td>432 (( \cdot \frac{2}{3} ))</td>
<td>256 (( \cdot \frac{2}{3} ))</td>
</tr>
<tr>
<td>( N_y )</td>
<td>196 (( \cdot \frac{2}{3} ))</td>
<td>320 (( \cdot \frac{2}{3} ))</td>
<td>192 (( \cdot \frac{2}{3} ))</td>
</tr>
</tbody>
</table>
results in two similar but distinct flow realizations, with different Reynolds numbers, form factors, skin-friction coefficients, etc.

In table 5.3, parameters of other simulations are listed for comparison. For his incompressible boundary-layer simulations, Spalart \[76\] employed extremely large domains, with a relatively large mesh spacing in the horizontal directions. Guarini \textit{et al.} \[28\], using a very similar method but adapted for compressible boundary layers, had to reduce the domain size so that they could have a smaller grid spacing. The incompressible channel-flow simulations of Moser \textit{et al.} \[54\] have resolution parameters very similar to the ones of Guarini and coworkers. The grid spacing in our nearly adiabatic simulations is still smaller by a factor of 2 to 3 than the one in Guarini \textit{et al.} \[28\], and it will be shown in the next sections that this is necessary for a proper spatial resolution. The sampling period $t_s$ (expressed in eddy turn-over times $\delta_0/u_\infty$) and the number of samples $n_s$ used to compute the statistics are found in table 5.2. Taking more samples would have helped to smooth some curves shown in the following chapters. However, the important features can very well be recognized and the costs (in time and computer resources) for further samples would have gone beyond the limits.

\begin{table}[h]
\centering
\caption{Parameters of experiments used for comparison (from \cite{22, 24}).}
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline
 & \textbf{Laderman} & & \textbf{Coles} & & \textbf{Mabey} & & \\
 & \textbf{7702S} & \textbf{7701S} & \textbf{5301} & \textbf{1301} & \textbf{1801} & \textbf{0502} & \\
\hline
\textbf{$M_\infty$} & 3.04 & 3.03 & 4.51 & 4.55 & 4.50 & 4.52 & 4.47 \\
\textbf{$T_w^* / T_\infty^*$} & 2.67 & 2.65 & 4.65 & 4.72 & 4.64 & 4.77 & 4.66 \\
\textbf{$Re_\delta_1$} & 17366 & 18557 & 35775 & 66431 & 30935 & 89398 & 32317 \\
\textbf{$Re_\delta_2$} & 1363 & 1476 & 880 & 1603 & 776 & 2310 & 1087 \\
\textbf{$Re_\theta$} & 3168 & 3411 & 3575 & 6601 & 3129 & 9522 & 4380 \\
\textbf{$C_f \cdot 10^3$} & 1.990 & 1.960 & 1.480 & 1.220 & 1.550 & 1.080 & 1.440 \\
\textbf{$u_r^* \cdot 10^2$} & 5.149 & 5.094 & 5.894 & 5.364 & 6.011 & 5.075 & 5.800 \\
\textbf{$\frac{u_r^*}{\nu_w^* \left[ \frac{1}{m} \right]$} & 52481 & 53151 & 19533 & 33380 & 39993 & 73009 & 19291 \\
\textbf{$\delta_0^+$} & 444 & 478 & 304 & 433 & 282 & 768 & 423 \\
\hline
\end{tabular}
\end{table}
5 Simulation parameters and results

fixed for this work.

Experimental data, mainly found in Fernholz & Finley [22, 24], are used to assess the quality of our numerical data. The main parameters of the chosen experiments are summarized in table 5.4. The comparison is often only possible for mean-flow data or integral values, turbulence statistics being more complicated to measure in the considered kind of flow.
Chapter 6

Influence of the wall temperature

The two simulations (T1, T2) discussed here were performed on the CRAY T3D in Lausanne with the method described in the preceding chapters. For both cases the free-stream Mach number \( M_\infty \) is 4.5 and the wall is isothermal. In the case T1 the laminar adiabatic wall temperature is imposed at \( z = 0 \), and four spatial steps have been performed. In the case T2, with five spatial steps, the wall temperature is reduced to one fourth of the value in T1.

6.1 Spectra and autocorrelations

The quality of the numerical resolution of the small scales can be assessed with one-dimensional Fourier spectra of the different flow variables. A rapid fall-off at high wavenumbers is a sign that the resolution is adequate since the magnitude of the approximation error of a spectrally represented quantity is comparable to the magnitude of the energy contained in the highest Fourier mode supported by the mesh.

Shown in figure 6.1 are the averaged one-dimensional spectra in \( x \) and \( y \) directions for the primitive variables \( \rho, u, v, w, T \) defined (for a flow quantity \( q \)) in \( x \) and \( y \) respectively as

\[
E_{q_x}(k_x, z) = \frac{1}{N_y} \sum_{j=1}^{N_y} \hat{q}(k_x, j, z) \hat{q}(k_x, j, z)^\dagger \quad (6.1)
\]

\[
E_{q_y}(k_y, z) = \frac{1}{N_x} \sum_{i=1}^{N_x} \hat{q}(i, k_y, z) \hat{q}(i, k_y, z)^\dagger \quad (6.2)
\]

where \( \hat{q} \) is the one-dimensional Fourier transform in the corresponding direction and the dagger \( \dagger \) denotes the complex conjugate. The spectra are
averaged in the other wall-parallel direction and in time (which is not indicated in the above formulae for clarity). If the spectrum amplitude decays of about three to four orders of magnitude between the lowest and highest wavenumbers then the numerical resolution is considered as sufficient, which holds here.

The computational domain is required to be large enough so that its length and width allow the turbulent fluctuations to decorrelate sufficiently and prevent the large-scale structures to interact with themselves. In figure 6.2 autocorrelation functions (averaged in space and time) are represented for the primitive variables in a given wall-parallel plane. Typically, the functions in $x$ show a quasi-monotonic decrease, while in the $y$-direction the
spanwise arrangement of some streamwise streaks is made visible by one or more marked negative minima. All functions are shown for a distance from the wall of about 20 wall units, but the effective distance is much smaller for the case T2. The fact, visible in all graphs, that the autocorrelation functions do not level off at zero near half the box length (or width) is due to the limited size of the computational domain. The cold-wall case T2, because of its larger computational domain in wall units, can accommodate more streamwise streaks. This reflects in the several local minima of the $y$-autocorrelation functions. This is also visible in the contour plots of the wall-normal vorticity $\omega_z = \partial v / \partial x - \partial u / \partial y$ shown in a horizontal plane close to the wall in figure 6.3. In both cases, the spanwise spacing of the

Figure 6.2: Autocorrelation functions; $\rho; \ldots \ldots \cdot u; \ldots \ldots \cdot v; \ldots \ldots \cdot w; \ldots \ldots \cdot T$; case T1 at $z^+ = 21$ in $x$-direction (a) and in $y$-direction (b); case T2 at $z^+ = 27$ in $x$-direction (c) and in $y$-direction (d).
streaks is approximately 100 wall units.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig6_3.png}
\caption{Contour plots of $\omega_z$ (a) case T1 in the plane $z^+ = 9$ (b) case T2 in the plane $z^+ = 10$. Flow from left to right.}
\end{figure}

6.2 Mean flow

Except for the fact that the streamwise variation is slow, no \textit{a priori} knowledge about the mean-flow behavior is needed with the ETDNS method. The following comparisons demonstrate that the computed mean flow matches experimental data favorably. Well documented cases are contained in the data compilations of Fernholz & Finley [22, 24], some of which have been used here to assess the quality of our numerical results. All relevant parameters of the considered experiments are presented in table 5.4. In figure 6.4(a) the mean profiles of the streamwise velocity $u$, streamwise momentum $\rho u$ and temperature $T$ of the case T1 agree well with data of Coles and Mabey. No experimental data were found with parameters matching the ones of
case T2. However, it can be seen that the strong temperature gradient at the wall is well resolved, the temperature maximum being at \( z/\delta_1 \approx 0.1 \) \((z^+ \approx 70, \text{beginning of the logarithmic region})\), figure 6.4(b). As recognized by Morkovin [52], the heat production through dissipation in the wall layer grows with \( M_\infty \) and easily overpowers effects of cooling at the wall, leading to a static temperature profile with a sharp maximum. The temperature remains below the one of the hot-wall case up to \( z/\delta_1 \approx 1.17 \) (end of the logarithmic region for both cases) and is then slightly larger approximately up to the boundary-layer edge where they both tend to one. Because of the smaller viscosity at the wall, the slope of the mean streamwise velocity profile at the wall is higher in the case T2, so that the skin-friction coefficient \( C_f \)

\[
C_f = 2 \frac{\mu}{Re} \frac{\partial \bar{u}}{\partial z} \bigg|_{w}
\]

is very similar for both the hot and cold-wall case. The hot-wall conditions tend to move the mass flux away from the wall, while a reduced wall temperature makes the \( x \)-momentum profile fuller close to the wall. At this free-stream Mach number \((M_\infty = 4.5)\) the difference between Reynolds-averaged values and Favre-averaged ones is quasi inexistent for \( u \) and very small for \( T \).
The van-Driest-transformed mean streamwise velocity profile $\tilde{u}_{VD}^+$ of a compressible boundary layer is defined as \([33]\)

$$\tilde{u}_{VD}^+ = \int_0^{\tilde{u}^+} \sqrt{\frac{\rho}{\rho_w}} \, d\tilde{u}^+$$  \hspace{1cm} (6.4)

with $\tilde{u}^+ = \tilde{u}/u_\tau$. The friction velocity $u_\tau$ is

$$u_\tau = \sqrt{\frac{\tau_w}{\rho_w}} \cdot$$  \hspace{1cm} (6.5)

The van Driest transformation accounts for the density variation across the boundary layer. It collapses compressible zero-pressure gradient boundary-layer profiles onto the law of the wall or logarithmic law \([73]\)

$$u^+ = -\ln z^+ + C$$  \hspace{1cm} (6.6)

where $\kappa$ is the von Kármán constant and $C$ a constant of integration. Equation (6.6) is formulated for the inner layer of zero-pressure gradient boundary layers with constant density. For $\tilde{u}_{VD}^+$, the same law applies in the form \([73]\)

$$\tilde{u}_{VD}^+ = \frac{1}{\kappa} \ln z^+ + C$$  \hspace{1cm} (6.7)

Fernholz & Finlcy \([23]\) suggest $\kappa = 0.40$ and $C = 5.1$ for turbulent boundary layers with zero-pressure gradient over an adiabatic wall. These “constants” are assumed to be largely independent of the Mach number and the Reynolds number \([73]\). However, the value of $C$ varies with the wall thermal boundary conditions. In the outer layer, a “law of the wake” or “defect law” can be formulated in a similar form for compressible flows \([21]\)

$$\tilde{u}_{\infty VD}^+ - \tilde{u}_{VD}^+ = -M \ln \left( \frac{z}{L} \right) - N$$  \hspace{1cm} (6.8)

where $L$ is an integral length defined as \([73]\)

$$\frac{L}{\delta_0} = \int_0^1 (\tilde{u}_{\infty VD}^+ - \tilde{u}_{VD}^+) \, d\left( \frac{z}{\delta_0} \right).$$  \hspace{1cm} (6.9)

For the Reynolds number range $1.5 \cdot 10^3 \leq Re_\theta \leq 4 \cdot 10^4$, an evaluation of a large number of experiments in zero-pressure gradient boundary layers, mainly along adiabatic walls, suggests $M = 4.70$ and $N = 6.74$ \([21]\).
As seen in figure 6.5(a), the case T1 follows the law of the wall quite well with a clear logarithmic region at $30 \lesssim z^+ \lesssim 100$. For the case T2 the additive constant of the logarithmic law is 7.6, but the slope is still given by $1/\kappa$. The logarithmic region is now found between $z^+ \simeq 100$ and 400. The outer region is much less sensitive to wall conditions and both cases follow the law (6.8) quite well in the region $0.09 \lesssim z/\mathcal{L} \lesssim 0.2$, figure 6.5(b). This is consistent with the measurements of Laderman [42] in a Mach 3 turbulent boundary layer at different wall temperatures, where the law of the wake is seen to be equally valid for all the tested wall-temperature lev-
Fernholz [21] had also recognized that the law of the wake (6.8) was equally valid for compressible turbulent boundary layers over isothermal walls with heat flux. As previously mentioned, the constants of equations (6.7) and (6.8) are based on experimental data. Figures 6.5(c) and (d) show how good the agreement is between these equations and experiments (cases from table 5.4). Obviously, the experimental scatter is larger than the deviations of the numerical results from the law of the wall and law of the wake.

6.3 Turbulence statistics

Different parameters have been defined to quantify compressible turbulence. One of the most commonly used is the turbulence Mach number $M_t$

$$M_t = \frac{\sqrt{u'^2 + v'^2 + w'^2}}{\bar{c}},$$

(6.10)

where $\bar{c} = \sqrt{T}/M_\infty$. Extensions of turbulence models for compressible flows use in their present form almost exclusively $M_t$. This suggests that strong turbulence fluctuations, e.g. of the magnitude of the speed of sound, produce compressibility effects strong enough to change the global turbulence properties [73]. In figure 6.6(a), the maximal value reached in both cases is larger than 0.3 (T1: 0.35, T2: 0.39), which seems to indicate that compressibility should have perceptible effects. The lower speed of sound in the wall region in case T2 causes the maximum turbulence Mach number to be larger than in the case T1. It is noteworthy that the numerator of equation (6.10) is 20% smaller in the cold wall case and closer to the wall than in the hot wall case (at $z = 0.03$ for T1 and $z = 0.02$ for T2, both in the respective buffer layer). A possible explanation for the reduced velocity fluctuations of case T2 is the larger inertia of the heavier fluid near the wall, which could damp the turbulent fluid movements. Note that this phenomenon can not be related to stabilization due to stratification caused by gravity, as the latter is ignored in the code and would be much smaller in comparison with other terms acting in the wall-normal direction. The higher viscosity near the hot wall is possibly responsible for the observed outward displacement of the $M_t$-maximum. The difference seen in the wake region (around $z \simeq 0.4$) is probably due to a lack of statistical convergence.
The fluctuating Mach number $M'$

$$M' = \text{rms}(M - \bar{M}),$$  \hspace{1cm} (6.11)

where $M = u/c$, is shown in figure 6.6(b). It takes into account the fact that both the velocity and the sound speed vary. Thus, according to Smits & Dussauge [73], $M'$ is larger than $M_t$. Furthermore, $M'$ develops a peak near the middle of the boundary layer where both the velocity and temperature fluctuations are important. Our data confirm this behavior and also show that the cold wall reduces the overall level of $M'$, since the static temperature fluctuations are smaller. However, the shape of the profile is similar for both cases.

Figure 6.7 shows that the static temperature fluctuations play a more important role in the second peak of $M'$ than the velocity fluctuations. The latter show a monotonically decreasing profile (very similar for both wall-temperature cases) while the former has a double-peak structure, more pronounced for the quasi-adiabatic case.

The profiles of the relative density fluctuations $\text{rms}(\rho')/\bar{\rho}$ have a shape very similar to the static temperature fluctuations. In the cold-wall case T2, the first maximum close to the wall is due to the large density gradient in that region, where the higher density makes it appear relatively small. The first extremum for the hot-wall case T1 is further away from the wall.
and is considerably larger than in the cold-wall case. Both cases show then a second extremum in the region $z \approx 0.5 \ldots 0.6$. In the major part of the boundary layer (except for the viscous sublayer), the density fluctuation level is lower in the cold-wall case. If the absolute fluctuations $\text{rms}(\rho')$ are considered, the global maximum is the one at $z \approx 0.6$, whose magnitude in the case $T1$ is by 40% larger than in the case $T2$.

### 6.3.1 Reynolds stresses and heat flux

The Reynolds normal stress $\bar{\rho} \bar{w}' \bar{w}''$ and Reynolds shear stress $\bar{\rho} \bar{w}' \bar{w}''$ are represented in figure 6.8(a) and (b). The normal stress has features similar to the ones of the turbulence Mach number $M_t$, though the smaller relative maximum is less pronounced. The latter is clearly visible in the shear stress for both cases and in the Reynolds heat flux $\bar{\rho} \bar{w}' \bar{T}''$ for the case with the quasi-adiabatic wall, figure 6.8(c). The much lower level of the Reynolds heat flux in the cold-wall case can be attributed to the smaller temperature differences across the boundary layer (except in the viscous sublayer and the buffer layer) and the damped velocity fluctuations. The negative portion of the curve near the wall is due to the positive wall-normal gradient of the mean static temperature.
Figure 6.8: (a) Reynolds normal stress (b) Reynolds shear stress (c) Reynolds heat flux; —— case T1. —— case T2.
6.3 Turbulence statistics

6.3.2 Reynolds analogy

One of the most widely used hypotheses for the analysis and computation of compressible boundary layers is Morkovin’s hypothesis. It was developed in 1962 by Morkovin [52] from an analysis of supersonic boundary-layer data, as they were available at that time. His conclusion was that for moderate Mach numbers (i.e. $M_\infty \lesssim 5$) "the essential dynamics of these shear flows will follow the incompressible pattern". This assertion is general and rather vague, but the consequences derived from this hypothesis include a scaling for velocity fluctuations and turbulent kinetic energy, and some particular forms of the Reynolds analogy for boundary layers on adiabatic flat plates. The hypothesis was used and reformulated by Bradshaw [9] to indicate that high-speed boundary layers can be computed using the same model as for low speeds by assuming that the density fluctuations are weak.

The similarity of the momentum and energy equations in an incompressible laminar boundary layer was recognized by O. Reynolds who could thus relate quantities pertaining to heat transfer with quantities pertaining to momentum transfer. This “Reynolds analogy” has then been used to describe approximate solutions in the compressible and turbulent cases that arise from assumed similarities between heat and momentum transfer.

Approximate solutions for compressible flows, which are coupled flows, require a complete set of equations (due to Young [87]) and the use of several assumptions to simplify them. Morkovin [52] suggested that Reynolds analogy might apply to compressible turbulence, a concept known as the strong Reynolds analogy (SRA). Later, other expressions of a Reynolds analogy have been formulated by several authors [27, 34]. Some of the proposed relationships are now considered in detail.

The mean momentum and mean total temperature equations for a stationary two-dimensional boundary layer with zero-pressure gradient in the streamwise direction can be written with the usual assumptions as [32, 27]

$$
\bar{\rho} \left( \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{w} \frac{\partial \bar{u}}{\partial z} \right) = \frac{\partial}{\partial z} \left( \frac{\bar{u}}{Re} \frac{\partial \bar{u}}{\partial z} - \bar{\rho} \bar{u}' \bar{w}' \right)
$$

(6.12)

\footnote{This expression is employed by Cebeci & Bradshaw [12] to characterize flows with large temperature differences where the temperature-field equations become nonlinear and are “coupled” to the velocity-field equations, since the viscosity and density depend on the temperature.}
\[
\tilde{p} \left( \tilde{u} \frac{\partial \tilde{T}_0}{\partial x} + \tilde{w} \frac{\partial \tilde{T}_0}{\partial z} \right) = \frac{\partial}{\partial z} \left( \frac{1}{\text{Pr} \text{Re}} \frac{\partial}{\partial z} \left( \tilde{T}_0 + (\text{Pr} - 1) \tilde{u}^2 \right) \right) \\
- \rho w'' T_0''.
\]

(6.13)

The total temperature is defined as

\[
T_0 = T + (\gamma - 1) M_\infty^2 \frac{u^2 + v^2 + w^2}{2}.
\]

(6.14)

Young [87] established a comparison between equation (6.12) and (6.13) in which he assumes that molecular effects are negligible while at the same time \( \text{Pr} = 1 \). Equations (6.12) and (6.13) have then the same form and their boundary conditions are analogous, that is

at the wall: \( \tilde{T}_0 - \tilde{T}_{0w} = 0 \) and \( \tilde{u} = 0 \),

at the free boundary: \( \tilde{T}_0 - \tilde{T}_{0w} = \tilde{T}_{0\infty} - \tilde{T}_{0w} \) and \( \tilde{u} = \tilde{u}_{\infty} \).

In the case of a heated or cooled wall (i.e. \( q_w \neq 0 \)) the following two solutions are admitted

\[
\tilde{T}_0 - \tilde{T}_{0w} = k_1 \tilde{u}
\]

(6.15)

\[
T_0'' = k_1 u''
\]

(6.16)

where \( k_1 \) is a constant derived from the conditions at the wall

\[
\bar{q}_w = -\frac{1}{(\gamma - 1) M_\infty^2 \text{Pr}} \left. \frac{\mu}{\text{Re} \text{Re}} \right|_w, \quad \bar{T}_w = \left. \frac{\mu}{\text{Re} \text{Re}} \right|_w.
\]

Morkovin [52] specifies \( k_1 \) in the form \( k_1^* = \text{Pr} \bar{q}_w (c_p^* \bar{T}_w^*) \) and calls (6.15) and (6.16) the strong Reynolds analogy. The determination of \( k_1 \) with the data set T2 was not conclusive: the “constant” \( k_1 \) varies strongly in the boundary layer and does not take the same values in equation (6.15) and (6.16).

If the wall is adiabatic, then \( k_1 \) vanishes and the two solutions become

\[
\tilde{T}_0 = \tilde{T}_{0w} = \text{const.}
\]

(6.17)

\[
T_0'' = 0 = T'' + (\gamma - 1) M_\infty^2 \tilde{u} u''
\]

(6.18)
stating that the total temperature is constant across the boundary layer and that total temperature fluctuations are zero. Morkovin [52] writes (6.18) as

\[ \sqrt{T_0''} = 0 \] (6.19)
\[ \sqrt{T''} = (\gamma - 1)M_\infty^2 \bar{u} \sqrt{u''^2} . \] (6.20)

In figure 6.9(a) equation (6.17) holds rather well for the quasi-adiabatic case T1. On the other hand, the predictions of equation (6.19) do not correspond to what is observed in the simulations. The total temperature fluctuations are of the same magnitude as the static temperature fluctuations in the quasi-adiabatic case T1, and even higher for the cold-wall case T2, figure 6.9(b).

\[ \text{Figure 6.9: (a) Total temperature } \bar{T}_0 \quad (b) \text{relative temperature fluctuations } \text{rms}(T'')/\bar{T} \text{ (thick lines) and } \text{rms}(T_0'')/\bar{T} \text{ (thin lines): --- case T1, -- -- case T2.} \]

Equation (6.20) can be rewritten in the form

\[ \frac{\sqrt{T''}}{T} \simeq 1 , \] (6.21)

which implies

\[ R_{u'' T''} = -1 , \] (6.22)
where $R_{u''T''}$ is the coefficient of correlation between $u''$ and $T''$

$$R_{u''T''} = \frac{u'' T''}{\sqrt{u''^2 \sqrt{T''^2}}} .$$

(6.23)

Experimental data support the validity of equation (6.21) in the non-intermittent zone $0.05 \leq z/\delta_0 \leq 0.7$, but the same is not true for equation (6.22) since $-R_{u''T''}$ differs from 1 by about 15 to 25% [27]. In figure 6.10, equation (6.21) performs quite well for case T1 in the region $z \geq 0.07$ (i.e. $z/\delta_0 \geq 0.1$). However, it fails completely for the cold-wall case T2.

The calculated correlation coefficient $R_{u''T''}$, shown in figure 6.11, does not follow the prediction of equation (6.22), which is not really surprising in view of the large total temperature fluctuations discussed above. Even in the quasi-adiabatic case T1 the magnitude of $R_{u''T''}$ is at most 0.85 close to the wall and decreases towards the edge of the boundary layer.

The highest values of $|R_{u''T''}|$ are close to the wall, where Antonia et al. [7] found that low-speed streaks coincide with high-temperature streaks and high-speed streaks with low-temperature streaks respectively.

The value of the correlation coefficient at the wall is highly dependent on the boundary conditions. The quasi-adiabatic case T1 shows a smaller $R_{u''T''}$ for $z = 0$ than the cold-wall case T2 with a larger temperature gradient near the wall. Note also in figure 6.11(b) the narrow region near
6.3 Turbulence statistics

![Figure 6.11: \( R_{u''T''} \) calculated (---) and predicted by equation (6.32) (-----) and equation (6.36) (- - -); (a) case T1, (b) case T2.]

the cold wall where the flow of case T2 shows a strong positive correlation between \( u'' \) and \( T'' \).

Using the turbulent Prandtl number \( Pr_t \), defined as

\[
Pr_t = \frac{\rho u'' w''}{\rho w'' T''} \frac{\partial \tilde{T}}{\partial z} \frac{\partial \tilde{u}}{\partial z},
\]  

(6.24)

Morkovin [52] proposed another SRA formulation obtained upon multiplying equation (6.18) by \( \rho w'' \), averaging the result and using the mean total temperature equation to replace \( \tilde{u} \)

\[
Pr_t \approx 1.
\]

(6.25)

In figure 6.12, the calculated turbulent Prandtl number, equation (6.24), varies considerably, but has a mean value in the boundary layer very close to 1. This also holds roughly for the case T2, although equation (6.25) was derived for flows over adiabatic walls.

Cebeci & Smith [13] used the Crocco relation between \( \tilde{u}, \tilde{T} \) and \( \tilde{T}_0 \) to derive from (6.16) an expression valid on heated or cooled walls

\[
\frac{\sqrt{T''^2/\tilde{T}}}{(\gamma - 1)M^2 \sqrt{u''^2/\tilde{u}}} \left( 1 + \frac{\tilde{T}_w - \tilde{T}_0}{\tilde{T}} \cdot \frac{\tilde{u}}{(\gamma - 1)M^2} \right)^{-1} \approx 1,
\]

(6.26)
Influence of the wall temperature

Figure 6.12: Turbulent Prandtl number $Pr_t$ calculated from equation (6.24) (solid) and predicted by equation (6.42) (dashed); (a) case $T_1$, (b) case $T_2$.

which is called "extended SRA" by Gaviglio [27]. This formulation shifts the curve of the basic analogy (6.21) for both cases $T_1$ and $T_2$ upwards without bringing it closer to 1 in a convincing way, figure 6.10.

Since the total temperature fluctuations are not significantly smaller than the static temperature fluctuations, the statement of a SRA is violated, as recognized by Morkovin [52]. However, experiments and numerical results show that equation (6.21) is very nearly satisfied for adiabatic walls, see figure 6.10(a). The question arises as to how this relationship can be satisfied if $\text{rms}(T'_0)$ is not negligible and of the same order as $\text{rms}(T'')$. Gaviglio [27] found that equation (6.19) gives a sufficient but not necessary condition for equations (6.20) through (6.22) to be valid. From the linearized definition equation for the total temperature fluctuations

$$T''_0 = T'' + (\gamma - 1) M^2 \bar{u} u'' ,$$

one finds after taking its square and averaging

$$\overline{T''_0^2} = \overline{T''^2} + (\gamma - 1)^2 M^4 \bar{u}^2 \overline{u''^2} + 2(\gamma - 1) M^2 \bar{u} u'' T'' .$$

The equation can be rearranged to give

$$\frac{\overline{T''^2} + (\gamma - 1)^2 M^4 \bar{u}^2 \overline{u''^2}}{\overline{T^2}} \approx 1 .$$

$$\frac{(\gamma - 1)^2 M^4 \frac{u''^2}{\bar{u}^2}}{\overline{T^2}} \approx 1 .$$
Comparing equation (6.29) with equation (6.21), one sees that (6.21) is valid if
\[ \overline{T''^2_0} \simeq 2 \left( \overline{T''^2} + (\gamma - 1) M_\infty^2 \overline{\tilde{u}'' T''} \right). \] (6.30)

The simulation data for our cases with quasi-adiabatic walls show that this condition holds rather well, except in the wall vicinity. Thus, the success of equation (6.21) is due to a fortuitous relationship between total and static temperature fluctuations rather than the assumption of negligible total temperature fluctuations [28].

If the validity of (6.20) (and (6.21)) is stipulated, it is possible to replace velocity fluctuations by temperature fluctuations in equation (6.28). Using the correlation coefficient \( R_{u'' T''} \), one gets
\[ \overline{T''^2_0} = 2 \overline{T''^2} + 2 \overline{T''^2} R_{u'' T''}. \] (6.31)

From (6.31), \( R_{u'' T''} \) can be expressed as a function of temperature fluctuations
\[ R_{u'' T''} = -1 + \frac{\overline{T''^2_0}}{2 \overline{T''^2}}. \] (6.32)

In case of negligible total temperature fluctuations, equation (6.32) reduces to Morkovin’s original equation (6.22). The predicted correlation coefficient of equation (6.32) compares well with the calculated \( R_{u'' T''} \) in the quasi-adiabatic case T1, see figure 6.11(a).

Gaviglio [27] proposes another relationship based on results involving the role of large-scale movements present in the boundary layer
\[ \frac{\sqrt{T''^2}}{T} \left( 1 - \frac{\partial \tilde{T}_0}{\partial T} \right) \simeq 1. \] (6.33)

This formulation would coincide with the SRA equation (6.21) in the case of a perfectly adiabatic wall. Furthermore, it takes into account a heat flux at the wall which provides a correction for the cold-wall case when compared to (6.21).

Huang et al. [34] point out that equation (6.33) is very similar to the expression derived by Rubesin [64]. Both can be written as
\[ \frac{\sqrt{T''^2}}{T} \left( 1 - \frac{\partial \tilde{T}_0}{\partial T} \right) \simeq 1, \] (6.34)
where \( A = 1.0 \) for Gaviglio and \( A = 1.34 \) for Rubesin. Noting that the factor \( A \) originates from mixing length considerations, Huang et al. show that it is approximately equal to the turbulent Prandtl number \( Pr_t \), giving

\[
\frac{\sqrt{T''u''^2}}{T} \cdot \frac{(\gamma - 1) \dot{M}^2 \sqrt{u''^2}}{\dot{u}} \cdot Pr_t \cdot \left(1 - \frac{\partial \tilde{T}_0}{\partial T}\right) \approx 1. \tag{6.35}
\]

They expect that equation (6.35) leads to errors of at least 20% if used to evaluate other velocity-temperature statistics, due to the fact that \( |R_{u''T''}| \) is lower than one (whereas (6.35) implies a correlation coefficient of unity). For case T1, neither equation (6.33) nor (6.35) bring a real amelioration compared to the original formulation (6.21), figure 6.10(a). Gaviglio’s expression gives an extremely wiggly profile, and Huang’s one fluctuates around unity. For the cold-wall case T2, the extended formulations (6.33) and (6.35) are performing much better than equation (6.21), though strongly fluctuating.

The value of \( R_{u''T''} \) predicted by the modified analogy of Huang et al. can be derived similarly to (6.32). Equation (6.35) can be substituted into equation (6.28) to obtain

\[
R_{u''T''} = \frac{\frac{T''u''^2}{T''u''^2} - 1}{2 Pr_t \left(1 - \frac{\partial \tilde{T}_0}{\partial T}\right)} - \frac{Pr_t}{2} \left(1 - \frac{\partial \tilde{T}_0}{\partial T}\right). \tag{6.36}
\]

This expression only does well in the outer half of the boundary layer \((z > 0.5)\) in the case T2 and it is less accurate than (6.32) in the quasi-adiabatic case, figure 6.11.

For the fact that experimental results with the hot-wire technique seem to agree much better with equation (6.22) than numerical data, Guarini et al. [28] give the following explanation. The experiments measure total temperature fluctuations, from which other values are derived. These fluctuations appear to be systematically smaller than the numerical ones by a factor of about two. Applying the relationships used to process the experimental data to their simulation data, with the total temperature fluctuations halved, Guarini et al. observe that the correlation coefficient \( R_{u''T''} \) rises to the level of the experimental data. They also notice that a factor-of-two error in the measurement of the total temperature fluctuations still gives good results for the rms-profiles of temperature and velocity fluctuations.

Morkovin was aware of the fact that the total temperature fluctuations are not negligible when compared to the static temperature fluctuations.
He stated [52] that another set of expressions could be derived by assuming that the correlation \( \rho w''T'' \) is much smaller than \( \rho w''T'' \). Our results show that this holds throughout the boundary layer in the quasi-adiabatic case T1, whereas in the cold-wall case T2 the above-mentioned assumption is satisfied only in the wake region. Multiplying the equation for the total temperature fluctuations (6.27) by \( \rho w'' \) and averaging gives

\[
\frac{\rho w''T''}{\rho w''T''} = \frac{\rho w''T''}{\rho w''T''} + (\gamma - 1) M_\infty^2 \bar{u} \frac{\rho w''w''}{2}.
\]

(6.37)

When \( \rho w''T'' \) can be neglected, one obtains

\[
\frac{\rho u''w''}{\rho w''T''} = -\frac{1}{(\gamma - 1) M_\infty^2 \bar{u}}.
\]

(6.38)

The Favre average of the total temperature can be written as

\[
\tilde{T}_0 = \tilde{T} + (\gamma - 1) M_\infty^2 \frac{\bar{u}^2 + \bar{v}^2 + \bar{w}^2}{2} + \frac{\rho u''w'' + \rho v''v'' + \rho w''w''}{2 \bar{\rho}}.
\]

(6.39)

On simplifying equation (6.39) by assuming that combinations of velocity fluctuations are small and the streamwise mean velocity is much larger than its spanwise and wall-normal counterpart, one gets

\[
\tilde{T}_0 = \tilde{T} + (\gamma - 1) M_\infty^2 \frac{\bar{u}^2}{2}.
\]

(6.40)

which becomes after differentiation:

\[
\frac{\partial \tilde{T}_0}{\partial z} = \frac{\partial \tilde{T}}{\partial z} + (\gamma - 1) M_\infty^2 \bar{u} \frac{\partial \bar{u}}{\partial z}.
\]

(6.41)

Substituting equation (6.41) in (6.38), one gets

\[
Pr_t \simeq \frac{\partial \tilde{T}}{\partial z} \frac{\partial \tilde{T}_0}{\partial z}.
\]

(6.42)

This expression agrees well with our simulation data in the inner portion of the boundary layer of case T1, where \( \rho w''T'' \) is stated above, figure 6.12(a). In the cold-wall case T2, \( \rho w''T'' \) is larger than \( \rho w''T'' \) for \( z \lesssim 0.3 \), so that equation (6.42) fails in this region.
6.3.3 Turbulent kinetic energy budget

The balance equation of the turbulent kinetic energy $\tilde{\rho}K$

$$\tilde{\rho}K = \frac{1}{2} \rho u_i u_i$$ (6.43)

in a compressible flow can be written as [26]

$$\frac{\partial \tilde{\rho}K}{\partial t} = - \frac{\partial}{\partial x_j} (\tilde{u}_j \tilde{\rho}K) + \tilde{\rho} \tilde{P} + \tilde{\rho} \Pi^{dt} + M +$$

$$+ \frac{\partial \tilde{\rho}}{\partial x_j} \tilde{D}_j + \tilde{\rho} \tilde{\epsilon} + \frac{\partial}{\partial x_j} \left( \frac{\tilde{\mu}}{Re} \frac{\partial K}{\partial x_j} \right).$$ (6.44)

The following interpretations can be assigned to the individual terms of equation (6.44): I – turbulence convection, II – turbulence production, III – pressure dilatation, IV – mass flux variation, V – turbulent diffusion, VI – turbulent dissipation, VII – viscous diffusion. Gatski [26] defines these terms as follows

$$\tilde{\rho} \tilde{P} = - \tilde{\rho} u_i u_i \frac{\partial \tilde{u}_i}{\partial x_j},$$ (6.45)

$$\tilde{\rho} \Pi^{dt} = \frac{\tilde{p}'}{\frac{\partial u_i}{\partial x_i}},$$ (6.46)

$$M = \frac{\tilde{u}_i}{\tilde{u}_i} \left( \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial \tilde{\rho}}{\partial x_i} \right),$$ (6.47)

$$\tilde{\rho} \tilde{D}_j = \frac{1}{2} \tilde{\rho} u_i u_i' u_j'' - \tilde{p}' u_i' \delta_{ij},$$ (6.48)

$$\tilde{\rho} \tilde{\epsilon} = \tau_{ij} \frac{\partial u_i}{\partial x_j}. $$ (6.49)

Our results show that the turbulence convection (I), pressure dilatation (III) and mass flux variation (IV) are very small, figure 6.13. The larger extrema for the turbulence production (II) and turbulent dissipation (VI) in the case $T_2$ are due to the higher density near the cold wall. If only $\tilde{\rho}$ and $\tilde{\epsilon}$ were plotted, they would have higher extrema in the hot-wall case. The higher value at the wall for the viscous diffusion (VII) in the cold-wall
case is caused by the very large temperature (and viscosity) gradients in \( z \) in that region. The strong density fluctuations near the cold wall make the \( z \)-profile of the mean wall-normal velocity component \( \bar{w} \) difficult to resolve numerically, as can be seen from the continuity equation. This is the origin of the fluctuations in the \( \bar{w}(z) \)-profile, which are visible in the convection term (1) for the case T2, further enhanced for the derivative \( \partial \bar{w}/\partial z \).

\[ 
\begin{align*}
\text{Figure 6.13: TKE budget according to equation (6.44), where all terms have been enlarged by a factor of 10^3;} & \quad \text{I, II, III, IV, V, VI, VII; (a) case T1, (b) case T2; zoom on curves I, III and IV; (c) case T1, (d) case T2.}
\end{align*}
\]
6.3.4 Intrinsic effects of compressibility

As stated by Lele [46], effects associated with the volume changes of fluid elements in response to changes in pressure are regarded as compressibility effects. These are contrasted with variable inertia effects associated with either variable composition or volume changes due to heat transfer.

If the viscosity fluctuations are neglected, the turbulent dissipation \( \bar{\rho} \epsilon \) can be split into a solenoidal \( \bar{\rho} \epsilon_s \), dilatational \( \bar{\rho} \epsilon_d \) and inhomogeneous \( \bar{\rho} \epsilon_I \) part [34]

\[
\bar{\rho} \epsilon = \bar{\rho} \epsilon_s + \bar{\rho} \epsilon_d + \bar{\rho} \epsilon_I
\]  

where

\[
\bar{\rho} \epsilon_s = 2 \frac{\mu}{Re} \frac{\Omega_{ij}' \Omega_{ij}'}{\partial x_i \partial x_j} \quad \text{with} \quad \Omega_{ij}' = \frac{1}{2} \left( \frac{\partial u_i'}{\partial x_j} - \frac{\partial u_j'}{\partial x_i} \right) \quad (6.50)
\]

\[
\bar{\rho} \epsilon_d = \frac{4}{3} \frac{\mu}{Re} \frac{\partial u_i'}{\partial x_i} \frac{\partial u_j'}{\partial x_j} \quad (6.51)
\]

\[
\bar{\rho} \epsilon_I = 2 \frac{\mu}{Re} \left( \frac{\partial^2 (u_i' u_j')}{\partial x_i \partial x_j} - 2 \frac{\partial}{\partial x_i} \left( u_i' \frac{\partial u_j'}{\partial x_j} \right) \right) \quad (6.52)
\]

Note that we use here \( u_i' \) and not \( u_i'' \), according to Huang et al. [34]. The differences between these fluctuations are in our cases very small. The dilatational dissipation \( \bar{\rho} \epsilon_d \) is called an explicit dilatational term. The ratios of \( \bar{\rho} \epsilon_d \) to \( \bar{\rho} \epsilon_s \) and \( \bar{\rho} \epsilon \) are plotted in figure 6.14(a). They are very small throughout the boundary layer, being less than 0.1% except in the region close to the wall where the maximal value is about 1%. For \( z \lesssim 0.35 \), the ratios are lower for the cold-wall case. There, both \( \epsilon_s \) and \( \epsilon_d \) are higher for the quasi-adiabatic case T1. The thick and thin curves are almost identical, showing that \( \epsilon_s \) is very close to \( \epsilon \) and both \( \epsilon_d \) and \( \epsilon_I \) are comparatively small. When the ratio \( \bar{\rho} \epsilon_d/\bar{\rho} \epsilon_s \) is plotted against the turbulent Mach number \( M_t \), figure 6.14(b), no sign of correlation is visible. This contrasts with the observation of Blaisdell et al. [8] who found that \( \epsilon_d/\epsilon_s \) is nearly proportional to \( M_t^2 \) in homogeneous shear flows.

Another term arising from the non-vanishing velocity divergence is the pressure-dilatation correlation \( \bar{\rho} \Pi_d \), equation (6.46). It represents a transfer between internal energy and turbulent kinetic energy. As seen in figure 6.13, this term is small compared to the relevant terms of the TKE budget.
6.3 Turbulence statistics

Figure 6.14: (a) Ratio of dilatational dissipation to solenoidal and total dissipation; thick line: $\bar{\rho} \Pi_{dl}/\bar{\rho} \epsilon_s$, thin line: $\bar{\rho} \Pi_{dl}/\bar{\rho} \epsilon$ (b) Ratio $\bar{\rho} \Pi_{dl}/\bar{\rho} \epsilon_s$ against the turbulent Mach number $M_t$ within the boundary layer (arrows indicate increasing $z$); —— case T1, ——— case T2.

Similarly to the channel-flow data of Huang et al. [34], $\bar{\rho} \Pi_{dl}$ is negative in the wall vicinity, where the magnitude of the extremum is higher in the cold-wall case. Indeed, the higher heat transfer at the wall drains more energy from the TKE.
Chapter 7

Influence of the Mach number

The three simulations discussed in this section were performed on a NEC SX-4/12 located at the Swiss Center of Scientific Computing (CSCS) in Mannhe. They are a continuation of the work initiated by Guo & Adams [29]. The considered turbulent boundary layers develop over isothermal walls at the respective laminar adiabatic wall temperatures. Since the turbulent heat fluxes at the wall turn out to be very small, we call these cases quasi-adiabatic. Four spatial steps have been performed in the cases M30 (with $M_{\infty} = 3.0$) and M45 (with $M_{\infty} = 4.5$), and five in the case M60 (with $M_{\infty} = 6.0$). The employed numerical algorithm is the one described in chapter 3, with the exception that the coordinate transform (term $Z_c$) is not used.

The structure of this chapter is very similar to the preceding one, and references will be made to formulas defined in chapter 6.

7.1 Spectra and autocorrelations

The averaged one-dimensional Fourier spectra for the primitive variables are shown in figure 7.1 for a height $z$ located in the respective buffer layer. A decay of three to four orders of magnitude is visible in all cases, indicating a correct resolution in the streamwise and spanwise directions. Note the upward shift with $M_{\infty}$ of the temperature curve, reflecting the temperature rise in the wall vicinity.

The averaged autocorrelation functions for the primitive variables are represented in figure 7.2 at the same height $z$ as the spectra. The limited extent of the computational domains prevents a perfect decorrelation of the fluctuations over half the domain length or width. In the streamwise direction, the density, streamwise velocity and temperature fluctuations decorrelate more slowly than the spanwise and wall-normal velocity fluctuations. The
7.1 Spectra and autocorrelations

Figure 7.1: One-dimensional Fourier spectra; $\rho$; $\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cd 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Figure 7.2: Autocorrelation functions; $\rho$; $\ldots, \ldots$ $u$; $\ldots, \ldots$ $v$; $\ldots, \ldots$ $w$; $T$; case $M30$ at $z^+ = 21$ in $x$-direction (a) and in $y$-direction (b); case $M45$ at $z^+ = 21$ in $x$-direction (c) and in $y$-direction (d); case $M60$ at $z^+ = 26$ in $x$-direction (e) and in $y$-direction (f).
same phenomenon is observed in the channel-flow simulation of Coleman et al. [14]. A special effort was done with the simulation M45, for which almost half the available memory capacity of the employed computer was necessary to accommodate the grid resolution. The increased size of the computational domain has not brought visible ameliorations for the autocorrelation functions, the curves keeping the same shape. Note that Guarini al. [28] also have problems to reach a zero autocorrelation for their streamwise velocity component in the streamwise direction near the middle of their domain, which is roughly twice as long as the one of case M45. The absolute minimum of the autocorrelation function for the wall-normal velocity \( w \) in the spanwise direction is an indication for the average width of the low-speed streaks found in the viscous sublayer, which is about 30 wall units. The (local) minimum of the \( u \)-autocorrelation function in the spanwise direction, located at roughly 50 to 100 wall units, corresponds to the mean spanwise spacing between streaks, which is in good agreement with experimental data [73]. For the case M45, this minimum is observed closer to the wall.

### 7.2 Mean flow

The mean profiles of the streamwise momentum \( \rho u \), streamwise velocity \( u \) and static temperature \( T \) are represented in figure 7.3 and compared with experimental data when available. For cases M30 and M45, the agreement with experiments is very good, in spite of the slight temperature mismatch at the wall. No data could be found to compare with case M60. In the considered Mach-number range, the difference between Reynolds average and Favre average for the streamwise velocity is negligible. However, the deviation between \( \overline{T} \) and \( \overline{T} \) is increasing with the Mach number. According to the definition,

\[
\overline{T} = \overline{T} + \frac{\rho' \overline{T}'}{\overline{\rho}}.
\]

Due to the large temperature difference between wall and free flow at higher \( \text{M}_\infty \), the negative correlation \( \rho' \overline{T} \) becomes important, showing that both density and temperature fluctuations augment. Another effect of increasing the free-stream Mach number, reflected in the transformation of the streamwise momentum profile, is the displacement of the bulk mass flow further
away from the wall, figure 7.3(d). The high-temperature, low-density region near the wall leads to a skewed mass-flux profile and a thicker boundary layer.

The van-Driest-transformed mean streamwise velocity profiles $\bar{u}_{V_D}$ are compared with the incompressible law of the wall in figure 7.4(a). The length of the logarithmic region is larger for cases with higher $Re_{\delta_2}$, such as M30. In the case M60, the buffer layer connects almost directly with the wake region. This holds also for the law of the wake, shown in figure 7.4(b),
7.3 Turbulence statistics

Figure 7.4: (a) Law of the wall: \( \bar{u}_{vD}^+ = z^+ \) and \( \bar{u}_{vD}^+ = 2.5 \ln z^+ + 5.1 \) (b) Law of the wake: \( \bar{u}_{\infty vD}^+ - \bar{u}_{vD}^+ = -4.70 \ln(z/L) - 6.74 \). M30, M45, M60.

where the logarithmic region of case M30 is more pronounced than in the two other cases.

7.3 Turbulence statistics

The maximum of the turbulence Mach number \( M_t \), figure 7.5(a), increases with \( M_\infty \) and slightly moves away from the wall. Huang et al. [34] find a maximum \( M_t \) of 0.35 (with definition equation (6.10)) for their channel flow at \( M = 3 \). In their simulation at \( M_\infty = 2.5 \), Guarini et al. [28] have a maximum \( M_t \) of 0.29, which is a little smaller than in our case M30 where \( M_{t_{max}} = 0.30 \). Their profile is fuller in the region \( z = 0.2\ldots0.3 \), similarly to our cases M45 and M60.

Morkovin [52] states that for \( M_\infty \) less than 5, one should not expect to find fluctuating Mach numbers \( M' \) greater than 0.2. In Spina et al. [79], a value of 0.3 is quoted at \( M_\infty \approx 4\ldots5 \). These assertions are not corroborated by our results, where the maximum \( M' \) goes from 0.31 for \( M_\infty = 3.0 \) up to 0.91 for \( M_\infty = 6.0 \), figure 7.5(b). Guarini et al. [28] also find a higher value (\( M'_{max} = 0.30 \)) at \( M_\infty = 2.5 \). With increasing \( M_\infty \), the \( M' \) profile develops a second extremum at \( z \approx 0.4 \), the first one being much closer to the wall (\( z \approx 0.03 \)). Around \( M_\infty = 5 \), the two extrema coexist with
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Figure 7.5: (a) Turbulence Mach number $M_t$ (b) fluctuating Mach number $M'$; case $M_{30}$, --- case $M_{45}$, --- case $M_{60}$.

approximately the same value, then the second one takes over. This outward displacement of $M'_{max}$ is confirmed by experimental results [73] and follows the appearance at the beginning of the wake region of a zone with high density and temperature fluctuations, illustrated in figure 7.6(b). Velocity fluctuations do not account much for the second extremum of $M'$, figure 7.6(a), as they monotonically decrease from their maximum near the wall.

7.3.1 Reynolds stresses and heat flux

For increasing $M_\infty$, the normal Reynolds stress $\bar{\rho} \bar{u}'' \bar{u}''$ shows a decreasing maximum located in the buffer layer, figure 7.7(a). This is a consequence of the diminishing mean density alone, since the maximum of the velocity fluctuations $\bar{u}'' \bar{u}''$ increases with $M_\infty$. The Reynolds shear stress, figure 7.7(b), reveals the same trend of decreasing fluctuations, however with an additional feature. For the higher Mach number case $M_{60}$, a second extremum appears at $z \approx 0.3$ in addition to the first one closer to the wall. It seems that this “double-peak” structure represent an intermediate state where the first peak (closer to the wall) has not yet disappeared while the second one is emerging. The strong density fluctuations appearing near the end of the logarithmic layer ($z \approx 0.4$) at higher $M_\infty$ is thought to be responsible for the appearance of the second peak of $\bar{\rho} \bar{u}'' \bar{u}''$, as well as the one of $M'$ seen
in figure 7.5(b).

This supports a suggestion of Morkovin [53], who says that the excess of the near-wall generated fluctuation energy diffuses outward to invigorate the outer turbulence, which would otherwise slowly decay. Owen & Horstman [58] proposed a similar theory for hypersonic boundary layers, where the turbulent fluctuations originating close to the wall propagate outwards as they are convected downstream. Another suggestion stems from the study of transition in compressible boundary layers. Adams [1] considers a coordinate system moving at the phase speed \( u_{ph} \) of the main perturbation wave, in which a relative sonic layer can be defined where the relative Mach number

\[
M_{rel} = M_{\infty} \frac{|\bar{u} - u_{ph}|}{\sqrt{T}}
\]  

(7.1)

is equal to one. This relative sonic layer divides the boundary layer into a relative supersonic \( (M_{rel} > 1) \) near-wall region and a relative subsonic \( (M_{rel} < 1) \) outer region, which are thus decoupled (see also Mack [48]).

For laminar or transitional compressible flows the general inflection point, where \( \partial (\bar{p} \partial \bar{u}/\partial z) / \partial z = 0 \) or \( \bar{p} \partial \bar{u}/\partial z \) has a local maximum, is located in the relative subsonic region and is responsible for inviscid instability. In our turbulent boundary layers the quantity \( \bar{p} \partial \bar{u}/\partial z \) shows a quasi-monotonic
Figure 7.7: (a) Reynolds normal stress (b) Reynolds shear stress (c) Reynolds heat flux; —— case M30, —— case M45, —— case M60.
7.3 Turbulence statistics

decrease for the lower Mach number, but reveals a clear local maximum around \( z \approx 0.35 \) at \( M_\infty = 6 \), figure 7.8. According to Robinson [62], instantaneously inflectional velocity profiles may roll up into vortices through a local shear-layer instability, even if the classic inviscid inflectional stability analysis assumes a steady two-dimensional flow. Thus, the second peak of the Reynolds shear stress at \( M_\infty = 6 \) could be related to an inviscid inflectional instability, the flow developing a "mixing-layer behavior" in the outer region, which is decoupled from the wall region through the presence of the relative sonic layer.

Experimental data are not of much help, as they scatter widely and do not show any clear trends. It is worth noting that if the Reynolds shear stress is represented without the density weight, i.e. as \( \overline{u''w''} \), then the extremum close to the wall prevails and the second one is almost smoothed out, so that the "double-peak" structure disappears (see section 8.1).

The increased level of temperature fluctuations around \( z \approx 0.4 \) can also be seen with the Reynolds heat flux, figure 7.7(c). Again, if the fluctuations are represented as \( \overline{w''T''} \) alone, one observes that the maximum for the higher Mach number cases moves closer to the wall, going from \( z \approx 0.3 \) down to \( z \approx 0.15 \).

\[ z \]

\[ 0 \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \]

\[ 0 \quad 0.5 \quad 1 \]

\( \overline{\rho \partial u / \partial z} \), normalized with its respective wall value; \( \ldots \ldots \) case M30, \( \ldots \ldots \) case M45, \( \ldots \ldots \) case M60, \( \ldots \ldots \) case T1, \( \ldots \ldots \) case T2.
7.3.2 Reynolds analogy

The cases considered here are all quasi-adiabatic, that is with a very small heat flux at the wall. The magnitude of their Stanton numbers

\[ St = \frac{\bar{q}_w}{\rho_w (T_w - T_\infty)} \]

is about $10^{-5}$. The mean total temperature $\bar{T}_0$ varies very little ($\pm 2\%$) above the logarithmic layer ($z \gtrsim 0.1$), figure 7.9(a). The difference between the free-stream $T_{0\infty}$ and wall total temperature $T_{0w} = T_w$ ranges from $0.10 T_{0\infty}$ for $M30$ to $0.15 T_{0\infty}$ for $M60$. For all considered $M\infty$, the SRA assumption of negligible total temperature fluctuations, equation (6.19), does not hold, as seen in figure 7.9(b) where the total temperature fluctuations have the same magnitude as their static counterparts.

Different SRA formulations are represented in figure 7.10. The original expression (6.21) performs rather well for all considered $M\infty$ in the mid boundary layer ($z \approx 0.2 \ldots 0.6$). The region close to the wall ($z \lesssim 0.2$) always shows a minimum lower than 1, and the fluctuations in the outer region ($z \gtrsim 0.6$) are no longer strong enough to produce reliable results. The trends observed for the curve of case M30 are similar to the results of Guarini et al. [28], except that their curve is smoother in the mid region.
Figure 7.10: SRA relations (left-hand side of the mentioned equations): \( (6.21), \quad (6.26), \quad (6.33), \quad (6.35); \) (a) case M30, (b) case M45, (c) case M60.
Figure 7.11: $R_{u''v''}$ calculated (— — —) and predicted by equation (6.32) (—— —) and equation (6.36) (−−−); (a) case M30, (b) case M45, (c) case M60.
Figure 7.12: Turbulent Prandtl number $Pr_t$ calculated from equation (6.24) (---) and predicted by equation (6.42) (----); (a) case M30, (b) case M45, (c) case M60.
The "extended SRA" of Cebeci & Smith (6.26) has the general tendency to shift the curve (6.21) slightly upwards, without really improving its behavior. The relationship of Gaviglio (6.33) gives slightly better results for $z < 0.2$, but produces unwanted fluctuations for higher $z$. The formulation (6.35) proposed by Huang gives the best results for $z \simeq 0.04 \ldots 0.4$, which corresponds to the end of the buffer layer up to the beginning of the wake region. All discussed formulas tend to very large values in the viscous sublayer, as the denominator of the common part (6.21) with the velocity and velocity fluctuations tends faster to zero than the numerator with the temperature fluctuations. Further, there is no visible Mach number effect affecting the validity of the above-mentioned formulas in the investigated Mach-number range.

The perfect anti-correlation between $u''$ and $T''$ predicted by the SRA (6.22) does not appear in the simulation results, figure 7.11, because of the non-negligible total temperature fluctuations illustrated in figure 7.9. For all cases, $R_{u''T''}$ reaches a minimum of about $-0.86$ at $z^+ \simeq 13$ (beginning of the buffer layer), then increases almost monotonically for higher $z$. The approximation formula for $R_{u''T''}$ (6.32), though very simple, gives very good results within the whole boundary layer, with the exception of the viscous sublayer. The formula (6.36) derived from the extended SRA formulation of Huang always slightly underestimates the magnitude of $R_{u''T''}$ by about 15% and has an erroneous behavior close to the wall.

The turbulent Prandtl number $Pr_t$, defined by equation (6.24) and represented in figure 7.12, fluctuates about 1. The fluctuations within the boundary layer may reach from +30% to −70%, while the results loose their meaning in the viscous sublayer. The constancy of $Pr_t$ stated by the SRA equation (6.25) seems not to depend on the free-stream Mach number, but rather on the quality of the turbulence statistics. Here, the case M45 is much smoother than M30 and M60.

### 7.3.3 Turbulent kinetic energy budget

The different terms of the balance equation of the turbulent kinetic energy (6.44) are: I - turbulence convection, II - turbulence production, III - pressure dilatation, IV - mass flux variation, V - turbulent diffusion, VI - turbulent dissipation and VII - viscous diffusion, see equations (6.45) to (6.49) for details. There is a clear order of magnitude separation between the dominant terms II, V, VI, VII and the secondary terms I, III, IV, figure
Figure 7.13: TKE budget according to equation (6.44), where all terms have been enlarged by a factor of $10^3$; ——— I, ——— II, ——— III, ——— IV, ——— V, ——— VI, ——— VII; (a) case M30, (b) case M45, (c) case M60; zoom on curves I, III and IV: (d) case M30, (e) case M45, (f) case M60.
The "stabilizing effect of compressibility" mentioned by Sarkar [68] for turbulent homogeneous shear flow is also visible in the present wall-bounded cases. The magnitude of the dominant terms diminishes with $M_\infty$, which is not only due to the decrease of the mean density in the wall region, as the same trend can be seen when the terms have been divided by the local mean density. The turbulence convection term depends largely on the wall-normal derivative of $\bar{\omega}$, which is a very sensitive quantity. The root-mean-square of the fluctuations $w''$ is one order of magnitude larger than the mean value $\bar{w}$ within the boundary layer, which makes it difficult to obtain a smooth profile for the mean wall-normal velocity component. Note that $\bar{w}$ and $\bar{\omega}$, both very small, have profiles with very different shapes within the boundary layer, whereas rms($w'$) and rms($w''$) are quasi-identical. Taking the $z$-derivative of $\bar{\omega}$ gives a still more critical value, which explains why no clear tendency can be seen for the curves I.

The pressure dilatation term III is negative in the wall region, and the magnitude of its extremum increases with $M_\infty$. However, it remains small in comparison with other terms and its spatial influence is limited to the viscous sublayer and beginning of the buffer layer. The mass flux variation term IV represents the influence of the mean pressure gradients and the mean shear stress gradients. It provides a small energy source for the TKE at the beginning of the buffer layer ($z^+ \approx 10$) and does not show a clear dependency on $M_\infty$.

### 7.3.4 Intrinsic effects of compressibility

The ratios of dilatational dissipation $\tilde{\rho} \epsilon_d$ to solenoidal ($\tilde{\rho} \epsilon_s$) and total ($\tilde{\rho} \epsilon$) dissipation are represented in figure 7.14(a) (see section 6.3.4 for the respective definitions). From $M_\infty = 3$ to 6 the ratio increases by roughly one order of magnitude. However, it remains small even for the case M60. The fact that thin and thick lines are very close shows that the solenoidal dissipation constitutes the dominant part of the total dissipation. There is no simple relationship between $\tilde{\rho} \epsilon_d / \tilde{\rho} \epsilon_s$ and the turbulence Mach number $M_t$, as seen in figure 7.14(b). Note that the relatively long and smooth part corresponding to $M_t \in [0, M_{t_{max}}]$ represents only the viscous sublayer and the first half of the buffer layer.

The pressure dilatation term $\tilde{\rho} \Pi^{dl}$, equation (6.46), is seen to grow with increasing free-stream Mach number in figure 7.13, but remains very small compared to the main terms of the TKE budget equation. Different models
have been developed for the pressure dilatation. For compressible isotropic turbulence with $M_t < 1$, Zeman [88] assumes that $\rho \Pi^{dl}$ is proportional to the rate of change of potential energy due to compression work. Sarkar [67] proposes for compressible sheared turbulence a model obtained from a formal solution for homogeneous turbulence. El Baz and Launder [19] modified the rapid part of the pressure-strain correlation to produce a model for compressible mixing layers which gives a finite pressure dilatation in the presence of either dilatational or shear strain. When applied to compressible boundary-layer flows, these models grossly over-predict the magnitude of $\rho \Pi^{dl}$. 

Figure 7.14: (a) Ratio of dilatational dissipation to solenoidal and total dissipation; $\rho e_d / \rho e_s$: thick line, $\rho e_d / \rho e$: thin line (b) Ratio $\rho e_d / \rho e$ against the turbulent Mach number $M_t$ within the boundary layer (arrows indicate increasing $z$); —— case M30, ——— case M45, ——— case M60.
Chapter 8

Discussion

8.1 Data normalization

If Morkovin's hypothesis holds, then a data scaling accounting for the mean property variations should successfully collapse the properly scaled compressible data onto the incompressible ones. One of these scalings is the van Driest transformation, equation (6.4), whose efficiency was demonstrated in the preceding chapters. Spina et al. [79] note that when the longitudinal velocity fluctuations are normalized by the shear velocity \( u_t \), there is a clear decrease in fluctuation level with increasing Mach number. However, when the streamwise normal Reynolds stress is normalized by the wall shear stress \( \tau_w = \rho_w u_t^2 \), the data exhibit some degree of similarity, particularly in the outer layer. Figure 8.1 shows that the density scaling brings the magnitude

![Figure 8.1:](image)

Figure 8.1: (a) Reynolds normal stress scaled with the wall shear stress \( \frac{\bar{w}''u''}{\tau_w} \); (b) Streamwise velocity fluctuations scaled with the shear velocity \( \frac{u''u''}{u_t^2} \); \( M30, ------ M45, ----- M60; Spalart [76]: + Re_\theta = 670, \times Re_\theta = 1410. \)
of the compressible extrema closer to the incompressible ones of Spalart [76]. However, the agreement is far from perfect and does not become better further away from the wall. With our results, the variation with \( M_\infty \) is smaller when the density scaling is not applied, figure 8.1(b), contrary to the observations of Spina et al. [79].

In our \( M_\infty = 4.5 \) cases, the density scaling clearly ameliorates the collapse of the profiles when the heat flux at the wall is important, particularly in the outer region, figure 8.2. However, it can not completely bring the extrema together.

![Figure 8.2: (a) Reynolds normal stress scaled with the wall shear stress \( \overline{\rho u'' w''}/\tau_w \); (b) Streamwise velocity fluctuations scaled with the shear velocity \( \overline{u''^2}/u^*_T \).](image)

We saw in section 7.3.1 that for higher Mach numbers the Reynolds shear stress profile \( \overline{\rho u'' w''} \) changes its shape and evolves towards a "double-peak structure". Interestingly, the new structure strongly depends on the density scaling, and it almost disappears when the shear stress is represented as \( \overline{u''^2}/u^*_T \), see figure 8.3. Besides, this normalization ameliorates the collapse of the curves.

Coleman et al. [14] mention the importance of accounting for the mean property variations in the near-wall scaling. For their compressible channel-flow simulations with cold walls, they compare the conventional wall variables (defined in terms of the mean density \( \rho_w \), viscosity \( \mu_w \), and shear stress \( \tau_w \) at the wall) with a semi-local scaling (replacing \( \rho_w \) with \( \overline{\rho(z)} \), \( \mu_w \) with \( \overline{\mu(z)} \) and \( u_T \) with \( u^*_T = \sqrt{\tau_w/\overline{\rho(z)}} \)). Coleman et al. observe a much better
collapse for velocity and vorticity fluctuations with the semi-local scaling. The improvement is not as clear for our nearly adiabatic cases, see figure 8.4. With the conventional wall scaling, all extrema lie between $z^+ \approx 12 \ldots 14$, but the curves scatter further away from the wall. The semi-local scaling does not improve the collapse of the curves, neither in the wall region nor in the outer region.

Figure 8.3: Favre averaged Reynolds shear stress $-\overline{u''w''}/u'^2$ (a) $\quad$ M30, $\quad$ M45, $\quad$ M60 (b) $\quad$ T1, $\quad$ T2.

Figure 8.4: Scaled Reynolds normal stress $\overline{\rho u''u''}/\tau_w$ (a) with classical wall scaling $z^+$ (b) with semi-local scaling $z^* = \bar{p} z u_*^* Re/\bar{\mu}$; $\quad$ M30, $\quad$ M45, $\quad$ M60; Spalart [76]: $+$ Re$_\theta = 670$, $\times$ Re$_\theta = 1410$. 
In figure 8.5 the locations of the maxima in cases T1 and T2 are not properly collapsed by the conventional wall scaling, whereas the semi-local scaling performs much better.

![Figure 8.5: Scaled Reynolds normal stress $\overline{\rho u' u'}/\tau_w$ (a) with classical wall scaling $z^+$ (b) with semi-local scaling $z^* = \rho z u'_* Re/\bar{\mu}$; $T1$, $T2$.]

Contrary to what has been seen with the Reynolds normal stress, the turbulence production $\rho \overline{P}$ of all our cases is well collapsed by the semi-local scaling in the near-wall region, figure 8.6. Originally, Spalart [76] used $u_\tau$,

![Figure 8.6: Normalized turbulence production $\rho \overline{P}/(\rho u'_*^4 Re/\bar{v})$ in semi-local scaling $z^* = \rho z u'_* Re/\bar{\mu}$; $M30$, $M45$, $M60$, $T1$, $T2$; Spalart [76]: $Re_\theta = 670$, $Re_\theta = 1410$.]

In order to normalize the Reynolds heat flux $\rho w''T''$, a reference temperature must be chosen. Huang et al. [34] propose to use the wall heat flux to define the friction temperature $T_\tau$ as follows

$$T_\tau = \frac{1}{\rho_w u_\tau Pr} \cdot \frac{\bar{\mu}}{Re} \cdot \frac{\partial \bar{T}}{\partial z} \bigg|_w .$$

They show that scaling $\overline{\rho w''T''}$ with $\rho_w u_\tau T_\tau$ is very successful to collapse their data. The observed success is probably mainly due to the fact that their channel has cooled walls, and thus a significant temperature gradient at the wall. In our nearly adiabatic cases, $T_\tau$ is very small ($\partial T/\partial z \to 0$) and the scaling fails, as seen in figure 8.7(a). For our cold-wall case T2, the scaled Reynolds heat flux reaches a maximum of 0.37, which is closer to the results obtained by Huang et al. but still remains roughly twice as large. An other possible reference temperature is the wall temperature $T_{w0}$.

Unfortunately, figure 8.8 shows that this choice also fails to collapse the data properly.

From a strictly dimensional reasoning, one finds a reference temperature $T_{ref}$ giving relatively good results for all our cases. We define $T_{ref}$ as being proportional to the squared friction velocity $u_\tau^2$ as

$$T_{ref}^* = \frac{u_\tau^*}{c_p^*} ,$$

\[ (8.2) \]
8.1 Data normalization

Figure 8.8: Scaled Reynolds heat flux $\frac{\rho w'' T''}{(\rho w_{ref} T_{ref})}$ (a) $M_{45}$, $M_{60}$ (b) $T_1$, $T_2$.

which gives in a non-dimensional formulation

$$T_{ref} = (\gamma - 1) M_{\infty}^2 u_r^2.$$ (8.3)

The agreement is not perfect, as seen in figure 8.9, nevertheless the quasi-adiabatic cases show less sensitivity to $M_{\infty}$. Also, the magnitudes of the maximal Reynolds heat fluxes for $T_1$ and $T_2$ are similar, even if the profiles have different shapes.

Figure 8.9: Scaled Reynolds heat flux $\frac{\rho w'' T''}{(\rho w_{ref} T_{ref})}$ (a) $M_{45}$, $M_{60}$ (b) $T_1$, $T_2$. 
8.2 Compressibility indicators

In the preceding chapters, the turbulence Mach number $M_t$ and the fluctuating Mach number $M'$ were presented, which are related to turbulence. Originally, they were considered (especially $M_t$) as "global" compressibility indicators, in the sense that if they exceeded a certain threshold value (say 0.3), compressibility effects would become important. This holds well for compressible isotropic turbulence, but as soon as mean shear is present, an additional "indicator" is needed to take its effects into account. The gradient Mach number $M_g$

$$M_g = \frac{S l}{\ddot{c}}$$

is usually used, where $S$ is the mean shear rate and $l$ a representative integral length scale in the direction of shear. Sarkar [68] demonstrated the importance of $M_g$ versus $M_t$ for compressible turbulent shear flows with a series of direct numerical simulations. He varied $M_t$ and $M_g$ separately and noticed that the stabilizing effect of compressibility on the turbulent energy growth rate is substantially larger in the simulation series where the initial value of $M_g$ is changed. Wall-bounded flows represent the next step of complexity, and reveal considerable differences in the intrinsic compressibility effects when compared with free shear flows. Sarkar [68] showed that the gradient Mach number in a high-speed boundary layer is very different from that in a high-speed mixing layer. In the logarithmic region of an adiabatic zero-pressure gradient flat-plate boundary layer, the mean shear rate is given by van Driest's scaling for the law of the wall

$$\frac{d\ddot{u}}{dz} = \frac{\sqrt{\tau_w/\ddot{p}}}{\kappa z}.$$  \hspace{1cm} (8.5)

With the wall distance $z$ as the appropriate integral length scale and the fact that the wall-normal mean pressure gradient practically vanishes, Sarkar derives

$$M_g = \frac{d\ddot{u}}{dz} \frac{l}{\ddot{c}} = \frac{M_\infty}{\kappa} \sqrt{\frac{C_f}{2}}.$$  \hspace{1cm} (8.6)

In the mixing layer, the maximum velocity gradient appears on the centerline and can be expressed by the mean velocity difference across the layer
(U_1 - U_2) and its thickness δ_{ML}(x), using an error-function type of velocity profile

\[ \frac{d\bar{u}}{dz} = 2 \frac{U_1 - U_2}{\sqrt{\pi} \delta_{ML}}. \] (8.7)

Approximating the integral length scale in the definition of M_g by \( l \simeq \delta_{ML} \), Sarkar gets

\[ M_g \simeq 2.2 M_c, \] (8.8)

where \( M_c \) is the convective Mach number

\[ M_c = \frac{U_1 - U_2}{c_1 + c_2}. \] (8.9)

This demonstrates that, when the reference Mach number is increased, the compressibility parameter \( M_g \) augments more rapidly in a mixing layer than in a boundary layer: \( M_g \) in a mixing layer with \( M_c = 1 \) is by one order of magnitude larger than \( M_g \) in the logarithmic layer of a supersonic boundary layer with comparable \( M_{\infty} \).

In figure 8.10, the general level of \( M_g \) increases with \( M_{\infty} \), while the wall temperature seems not to influence much the shape of the profile. For all our cases, \( M_g \) has two main local maxima, the first one in the buffer layer at \( z \simeq 0.02 \ldots 0.04 \) and the second one at \( z \simeq 0.4 \ldots 0.6 \), which becomes the

![Figure 8.10: Gradient Mach number M_g](image)

\( M_30, \overline{\ldots \overline{\ldots}} M_45, \overline{\ldots \overline{\ldots}} M_60, \overline{\ldots \overline{\ldots}} T_1, \overline{\ldots \overline{\ldots}} T_2. \)
largest one for higher $M_{\infty}$. The values computed with equation (8.6) in the logarithmic region (around $z \approx 0.1 \ldots 0.2$) are local minima, but even the global maxima are still smaller than the values reached in a corresponding mixing layer. Note that once again, the cases with higher Mach numbers are characterized by an enhanced activity in the mid boundary-layer region.

Thus, the low level of intrinsic compressibility effects such as the dilatational dissipation or the pressure-dilatation correlation in our wall-bounded flows up to Mach 6 may be related to the smallness of the gradient Mach number, even if the turbulence Mach number assumes relatively large values. Note that $M_g$ is based only on integral or mean values, and it would be interesting to have a compressibility indicator constructed with turbulent quantities. Friedrich & Bertolotti [25] show that in homogeneous turbulent shear flows, there is a direct coupling between the velocity fluctuations in direction of the mean shear (in our case $z$) and dilatation fluctuations. This implies that a damping of $w'$ also reduces $\partial u'_i/\partial x_i$. Of course, such a direct and simple coupling does not exist for wall-bounded flows, where the mean shear $\partial \bar{u}/\partial z$ is a function of $z$. However, the idea could be useful to develop a new compressibility indicator based on $w'$, for example a transverse Mach number $M_{tr}$ defined as

$$M_{tr} = \frac{\sqrt{w'^2}}{c}. \quad (8.10)$$

![Figure 8.11: Transverse Mach number $M_{tr}$ (a) $M_{30}$, (b) $M_{60}$, $M_{45}$, $T_1$, $T_2$.](image-url)
In figure 8.11, this transverse Mach number is seen to be relatively small, but increases with $M_\infty$. It is practically not influenced by the wall temperature.

### 8.3 Anisotropy tensor

Usually, the intrinsic compressibility effects on turbulence structure are described in terms of magnitude of the dilatational dissipation or the pressure-dilatation correlation, i.e. quantities which can differ from zero only in compressible flows. However, some authors (like Sarkar [68], Smits & Dussauge [73]) suggest that the first signs of compressibility effects are indicated by changes in the anisotropy of the Reynolds stresses. The Reynolds stress anisotropy tensor $b_{ij}$ is defined as

$$b_{ij} = \frac{u_i' u_j'}{u_k' u_k'} - \frac{1}{3} \delta_{ij} \ .$$

The DNS data of Sarkar [68] for turbulent homogeneous shear flows clearly show that the Reynolds stress anisotropy tensor strongly depends on $M_g$ and much less on $M_t$. For $M_g$ going from 0.22 to 1.32, $b_{13}$ varies from $-0.15$ to $-0.06$, $b_{11}$ from 0.32 to 0.60 and $b_{33}$ from $-0.20$ to $-0.30$. The reduction in the Reynolds shear stress anisotropy $b_{13}$ and consequently a reduction of the turbulence production level is predominantly responsible for the reduced growth rate of the turbulent kinetic energy. Sarkar also notes that the “dilatational terms” (pressure dilatation and dilatational dissipation) are not negligible in the sense that they are as large as 20% of the TKE budget, but they do not cause the observed reduction of the growth rate. The compressible data of Blaisdell et al. [8] lie within the range of Sarkar’s results. The incompressible data of Rogers et al. (cited in Speziale et al. [78]) confirm the trend of Sarkar’s data with $b_{13} = -0.158$, $b_{11} = 0.215$ and $b_{33} = -0.153$.

For the mixing layer, Vreman et al. [84] find that $b_{11}$ increases from 0.05 to 0.25 when $M_e$ varies from 0.2 to 1.2. They show that the reduced pressure fluctuations are responsible for the changes in growth rate via the pressure-strain term, in particular its “rapid” components. Meanwhile, the increase of $b_{11}$ at high Mach numbers limits the growth rate reduction through the “slow” pressure-strain term. Ladeinde et al. [41] find for their two-dimensional mixing layer that $b_{13}$ varies from roughly $-0.24$ to $-0.12$ when $M_e$ increases from 0.5 to 1.0 (short time behavior, i.e. for approximately the
first 20 non-dimensional time units). They observe that the results of their study and Sarkar's one [68] are quite similar in terms of TKE growth rate and anisotropy tensor, despite the different initial and boundary conditions of both problems.

The possible dependence of $b_{ij}$ on a Mach number is difficult to assess with the available data for wall-bounded flows, either because the investigated Mach number range is too small or because there is no such dependence in this kind of flow. Mazouz et al. [49] have investigated experimentally an incompressible channel flow. In their measurements, $b_{11}$ varies from 0.30 near the wall down to 0.15 at the centerline, while $b_{33}$ decreases from $-0.2$ to $-0.1$. This agrees well with the experimental results of Laufer (cited in Speziale [77]) who obtained in an incompressible channel flow the following equilibrium values in the logarithmic layer: $b_{11} = 0.22$, $b_{22} = -0.07$, $b_{33} = -0.15$ and $b_{13} = -0.16$. In the compressible boundary layer at Mach 3 and $Re_\theta = 84000$ of Konrad & Smits [40], the measured $b_{13}$ decreases from $-0.12$ near the wall to $-0.07$ at the boundary-layer edge.

The components of the anisotropy tensor for our simulations are illustrated in figure 8.12 together with the incompressible boundary-layer data of Spalart [76] and channel-flow data of Moser et al. [54]. For each component, independently of the Mach number, wall condition or type of flow (channel or boundary layer), the different curves are very similar. In the logarithmic region, which corresponds to $z \approx 0.2 \ldots 0.3$, we find $b_{11} \approx 0.1 \ldots 0.2$, $b_{22} \approx -0.03 \ldots -0.07$, $b_{33} \approx -0.10 \ldots -0.16$ and $b_{13} \approx -0.13 \ldots -0.18$. Smits & Dussauge [73] state that the anisotropy depends strongly on the Reynolds number. This surely holds for fluctuations of velocity components taken separately (like $\bar{w}'^2$, $\bar{v}'^2$), but this does not correspond to our observations as far as the anisotropy tensor is concerned. The compressible boundary layer of Konrad & Smits [40] with $Re_\theta \approx 84000$ has $b_{ij}$ values in the logarithmic region very similar to our cases with much lower Reynolds numbers. These authors however mention considerable measurement uncertainties with their crossed-wire technique (typically more than $\pm 10\%$). We also note that the values of $b_{ij}$ for wall-bounded flows in the logarithmic region are quite close to the ones of a turbulent homogeneous shear flow at $M_g \simeq 0.2$ or a mixing layer at $M_c \simeq 1.0$ (which would correspond with equation (8.8) to $M_g \simeq 2.2$). Looking back at figure 8.10 and comparing the behavior of $M_g$ with the one of the components of $b_{ij}$ in figure 8.12, one notices that the gradient Mach number varies by about $\pm 30\%$ to $\pm 50\%$. 


between \( z \approx 0.2 \) and 0.6, while the anisotropy tensor remains approximately constant. The interpretation of this observation can be twofold. On the one hand, it is possible that for wall-bounded flows larger variations or absolute values of \( M_g \) are required to make a change in the anisotropy tensor visible, perhaps together with a higher Reynolds number. On the other hand, the gradient Mach number might not be an adequate indicator for wall-bounded flows, or needs to be supplemented by a further parameter, see section 8.2.

The invariants \( \Pi \) and \( \Pi_3 \) of the Reynolds stress anisotropy tensor are defined as [47]

\[
\Pi = -\frac{1}{2} b_{ij} b_{ji} \tag{8.12}
\]
All possible anisotropy states are bound to a finite region in the $II$, $III$ plane, the so-called anisotropy-invariant map (AIM), delimited by three boundary lines illustrated in figure 8.13. The upper boundary is the locus of two-dimensional states and the two sides are the two types of axisymmetric states (axisymmetric contraction ($III < 0$) and expansion ($III > 0$)). The upper vertex is the one-dimensional state and the origin represents the isotropic state. The paths of anisotropy states for all our cases are represented in figure 8.13, where data of the incompressible boundary layer of Spalart [76] at $Re_\theta = 1410$ are included for comparison. All paths follow approximately the same pattern, which can be defined as follows for increasing $z$. Close to the wall, turbulence is two-dimensional. Because of the strong mean shear, it moves then along the 2D-line towards the one dimensional state, to which it is the closest in the mid buffer layer. Subsequently, the path follows the line of axisymmetric expansion towards the origin, and ends very close to an isotropic state at the the boundary layer edge. With the available data, it was not possible to determine any clear influence of the Mach number, the Reynolds number or the wall temperature on the shape.

\[ III = \frac{1}{3} b_{ij} b_{jk} b_{ki}. \]  

(8.13)

---

**Figure 8.13:** Anisotropy-invariant map. Turbulence must occur within the region (or on its boundaries) delimited by the axisymmetric ($III = \pm \left(-\frac{II}{3}\right)^{3/2}$) and two-dimensional ($\frac{1}{6} + 3III + II = 0$) states (dotted lines). Arrows indicate the direction of increasing $z$. (a) $M30$, $M45$, $M60$, $\times$ Spalart [76] with $Re_\theta = 1410$; (b) $T1$, $T2$. 


8.4 Forcing terms

The key features of the ETDNS method are the forcing terms, which "reconstruct" the streamwise development of the mean flow, see chapter 2. In the simulations T1 and T2, equation (2.2) was solved, while in the other simulations the term $Z_c$ in (2.2) was not implemented for consistency reasons ($Z_c$ was not implemented in the code that Guo & Adams [29] used to initiate the simulations M30, M45 and M60). The way the different forcing terms act on the flow is illustrated in figures 8.14 and 8.15 for our two cases at $M_\infty = 4.5$, T1 and M45. Represented are the terms on the right-hand side of equation (2.2) at a time instant at the end of the sampling period, averaged in the homogeneous directions $x$ and $y$. In this section, this spatial averaging is denoted with an overbar $\overline{\bullet}$.

The largest extrema of the averaged flux derivatives and forcing terms are found for the streamwise momentum $\rho u$, the density $\rho$ and the total energy $E$. The corresponding terms for $\rho v$ and $\rho w$ are one order of magnitude smaller. Interestingly, these dominant variables $\rho u$, $\rho$ and $E$ display forcing term profiles with a high degree of similarity, probably due to the strong influence of $\partial \overline{\rho u}/\partial X$ which is present in all the respective components. The term $\overline{Z_1}$, equation (2.33), is negligibly small compared to the other forcing terms. The sum of the flux derivatives $\partial \overline{F}/\partial x + \partial \overline{G}/\partial y + \partial \overline{H}/\partial z$ is seen to be of approximately equal magnitude but opposite sign to $Z_0$. The term $Z_c$ is small and mainly plays a role where $Z_0$ is maximum, that is near $z \approx 0.5$. We have not observed noticeable differences in the results due to $Z_c$. The somehow dissimilar shapes observed for corresponding terms in T1 and M45 (like the local maximum of $Z_0$ near $z \approx 0.2$ for $\rho$, $\rho u$ and $E$ in T1) come rather from the different flow histories than from the presence (or absence) of $Z_c$. $Z_0$ and $Z_c$ are mainly positive and thus represent source terms for the time evolution of the conservative variables, the energy supplied by the slow scales. It is interesting to note that the mid boundary layer region ($z \approx 0.4 \ldots 0.5$), where an increase of turbulent activity was observed (see sections 6.3 and 7.3), is where the sum of the averaged flux derivatives and $Z_0$ of the dominant variables ($\rho u$, $\rho$, $E$) reach their maximal magnitude. Also, the maximum of $\text{rms}(\langle \rho u \rangle')$ is reached precisely in that region.
Figure 8.14: Spatially averaged terms of the governing equation (2.2) for case T1; sum of averaged flux derivatives; \(-\cdots\) $Z_0$; \(-\cdots\) $Z_1$; \(-\cdots\) $Z_0$; (a) first solution component $\rho$ (b) second solution component $\rho u$ (c) third solution component $\rho v$ (d) fourth solution component $\rho w$ (d) fifth solution component $E$. 
Figure 8.15: Spatially averaged terms of the governing equation (2.2) for case M45; sum of averaged flux derivatives; \( Z_0 \); \( Z_1 \): (a) first solution component \( \rho \) (b) second solution component \( \rho u \) (c) third solution component \( \rho v \) (d) fourth solution component \( \rho w \) (d) fifth solution component \( E \).
8.5 Possible improvements

The following considerations are some a posteriori reflections, inspired by the experience gained with the different simulations. Though the code in the form described here was seen to perform well and give very valuable results, it appears that a couple of points could be ameliorated.

The formulation of the energy equation with the total energy $E$ in the conservative form implies frequent transforms in order to calculate the primitive variables $p$ and $T$,

$$p = (\gamma - 1) \cdot \left( E - \frac{1}{2} \rho \left( u^2 + v^2 + w^2 \right) \right)$$

$$T = \gamma(\gamma - 1) M_\infty^2 \left( \frac{E}{\rho} - \frac{u^2 + v^2 + w^2}{2} \right).$$

These operations involve the triple products $\rho u_i^2$ which are prone to generate aliasing errors, for example in the wall-normal direction near the boundary-layer edge where the grid resolution could be marginal. Note that a high-order filter was employed to cope with that aspect (see section 3.1.2). However, a formulation of the energy equation with primitive variables would contribute to reduce the above-mentioned problem. If the static pressure $p$ is taken as new variable, the equation to be solved is then

$$\frac{\partial p}{\partial t} = - \frac{\partial (pu_j)}{\partial x_j} - (\gamma - 1) p \frac{\partial u_j}{\partial x_j} + (\gamma - 1) \frac{\partial q_j}{\partial x_j} + (\gamma - 1) \tau_{ij} \frac{\partial u_i}{\partial x_j}. \quad (8.16)$$

As the flux formulation can no longer be employed, the structure of the corresponding forcing terms also changes, for instance in $Z_0$ and $Z_1$

$$Z_0|_{\text{energy}} = - \frac{\partial (pu)}{\partial X} + (\gamma - 1) p \frac{\partial \bar{u}}{\partial X} +$$

$$\left( \frac{4}{3} \left( \frac{\partial \bar{u}}{\partial X} \right)^2 + \frac{\partial \bar{v}}{\partial X} \frac{\partial u}{\partial y} + \frac{\partial \bar{w}}{\partial X} \frac{\partial u}{\partial z} \right). \quad (8.17)$$

$$Z_m|_{\text{energy}} = \frac{1}{PrM_\infty^2} \frac{\partial}{\partial X} \left( \frac{\bar{\mu}}{Re} \right) \frac{\partial \bar{T}}{\partial X} +$$

$$\left( \frac{4}{3} \left( \frac{\partial \bar{u}}{\partial X} \right)^2 + \frac{\partial \bar{v}}{\partial X} \frac{\partial u}{\partial y} + \frac{\partial \bar{w}}{\partial X} \frac{\partial u}{\partial z} \right) - \frac{2}{3} \frac{\partial \bar{u}}{\partial y} \frac{\partial v}{\partial X} +$$

$$\frac{2}{3} \frac{\partial \bar{u}}{\partial z} \frac{\partial v}{\partial X}.$$
8.5 Possible improvements

\[
\left( \frac{\partial \bar{\nu}}{\partial X} \right)^2 - \frac{2}{3} \frac{\partial \bar{u}}{\partial X} \frac{\partial \bar{w}}{\partial z}, \quad (8.18)
\]

\[
Z_1 \bigg|_{\text{energy}} = -(p - \bar{p}) \frac{\partial \bar{u}}{\partial X} - (u - \bar{u}) \frac{\partial \bar{p}}{\partial X}. \quad (8.19)
\]

The structural changes for \( Z_e \) are larger and not treated here. Note that the wall boundary conditions for \( p \) can still be expressed as a function of the given wall temperature \( T_w \) and the calculated density \( \rho \) as

\[
p(x, y, z = 0) = \frac{1}{\gamma M_\infty^2} \rho(x, y, z = 0) T_w. \quad (8.20)
\]

A considerable advantage of the formulation (8.16) is that the triple products \( \rho u_i^2 \) are no longer needed to compute \( p \). Also, the static pressure, which is a very sensitive value, is computed directly as solution of a PDE system and can thus be better controlled (wall boundary conditions, filtering). The price of this modification is then a different structure for the energy component of the forcing terms \( Z_0 \) and \( Z_1 \), while the corresponding part of \( Z_e \) should undergo deeper changes.

A flat-plate boundary layer with zero-pressure gradient is expected to have a two-dimensional mean flow, in the sense that the mean spanwise velocity component is zero. In our code, nothing is done to enforce that

---

Figure 8.16: Mean profile of the spanwise velocity component \( \bar{v} \) normalized with the maximal rms fluctuation value \( \max \left( \sqrt{v''^2} \right) \):

- \( - - - M30, - - - M45, \)
- \( - - - M60, \)
- \( \cdots \) \( T1, \) \( - - - T2. \)
condition and \( \tilde{v} \) develops without any corrections. Note however that the laminar mean flow of the transition simulations used as initial conditions (see section 2.5) is strictly two-dimensional. The mean spanwise velocity profiles for all our cases are represented in figure 8.16, normalized with the respective maximal value of \( \text{rms}(v'') \). This illustrates the "unforced" evolution of \( \tilde{v} \) after four or five spatial steps (i.e. typically 400 to 900 time units of turbulent calculation) and one observes that the mean flow has become like stratified, with layers drifting slowly in positive or negative spanwise direction. Though \( \tilde{v} \) remains very small in comparison with \( \tilde{u} \) (\( \tilde{v}_{\text{max}} \) is at the most 0.8% of \( \tilde{u}_{\text{max}} \)), some extrema are seen to exceed 20% of the corresponding maximal \( \text{rms}(v'') \). The origin of the profile evolution lies in some aliasing and rounding errors, which accumulate with time without being corrected. Thus, it would be physically absolutely justified to enforce \( \tilde{v} = 0 \) during the time advancement. Further, this measure could improve the quality of the turbulence statistics \(^1\).

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\(^1\)After completion of this work, the above-mentioned measure was implemented and tested. First results indicate that the main effect of setting \( \rho \tilde{v} \) to zero is a small increase of the streamwise velocity fluctuations \( u' u' \) in the region \( z \approx 0.3 \).
Chapter 9

Conclusions and recommendations

An extended temporal DNS (ETDNS) method was employed to simulate spatially developing turbulent flat-plate zero-pressure gradient boundary layers over isothermal walls in the supersonic regime. The considered free-stream Mach numbers $M_\infty$ range from 3 to 6, the Reynolds numbers based on the respective momentum thickness and free-stream viscosity $Re_\theta$ lie around 3000, and the wall is either nearly adiabatic or strongly cooled.

With the ETDNS method, based on the classical temporal approach, it is possible to reconstruct the streamwise development of the mean flow and thus to incorporate the mean-flow streamwise gradients into the underlying Navier-Stokes equations as forcing terms. The computational domain is chosen just large enough to let the turbulent fluctuations decorrelate sufficiently over its length and width. It is marched stepwise downstream during the computation, thus describing the mean boundary layer evolution over the considered streamwise extent in a discrete way. Among the three employed forcing terms, the largest and most important is the one representing the effects of mean-flow non-parallelity on the mean flow itself ($Z_0$). The term related to a coordinate transformation ($Z_c$) is one order of magnitude smaller, and the one describing the interaction of the mean-flow non-parallelity with the turbulent fluctuations ($Z_1$) still one order of magnitude smaller. Compared with a fully spatial simulation, the ETDNS reduces the computational effort by one to two orders of magnitude due to the smaller computational domain and the possibility of averaging in the streamwise direction when computing the turbulence statistics.

Computations were performed on two parallel computers with different architectures. The explicit parallelization of the code and subsequent optimization for a CRAY T3D massively parallel computer is described. The porting of the code onto a NEC SX-4 vector parallel machine allowed for the comparison of the code performances on both architectures. The explicit
parallelization has the advantage of transparency for the data distribution and data passing between the processors, is however time-costly. The massively parallel machine had a larger memory capacity, but it was impossible to reach more than roughly 10% of the peak performance on one processor (averaged code performance) while about 50% was obtained on the vector parallel machine.

The ETDNS method has proven to be a valuable tool for the investigation of compressible turbulent boundary layers. The results obtained after four to five marching steps closely match experimental mean-flow data, where the only *a priori* assumption made about the mean-flow development is the fact that it is slow.

None of the expected "high Reynolds number effects" was found near the strongly cooled wall of a $M_\infty = 4.5$ boundary layer. In spite of the relatively low local viscosity, the velocity fluctuations are smaller than for a nearly adiabatic wall, as are the static temperature fluctuations. The total temperature fluctuations are larger for the cold wall case due to the strong heat transfer at the wall. Apart from this exception, it seems that a reduction of the wall temperature generally results in a decrease of the fluctuations with no significant changes in the turbulence structure. Note that the large mean temperature and density gradients at the cold wall have been well resolved.

In boundary-layer flows with small wall heat flux, the classical compressibility indicators become relatively large with increasing free-stream Mach number: The maximal turbulence Mach number $M_t$ exceeds 0.4 and the fluctuating Mach number $M'$ reaches 0.9 at $M_\infty = 6$. However, intrinsic compressibility effects (dilatational dissipation and pressure-dilatation correlation) are small, though they increase with $M_\infty$. The gradient Mach number $M_g$ is found to be much smaller in a supersonic boundary layer than in a mixing layer with comparable convective Mach number.

The fact that the van-Driest-transformed velocity profiles compare well with the incompressible law of the wall, that the anisotropy tensor has approximately the same values for compressible and incompressible boundary layers, and that the intrinsic compressibility effects remain small tends to support Morkovin's hypothesis. However, we have observed that for $M_\infty \gtrsim 5$ the relative density fluctuations become important in the outer part of the boundary layer, causing the Favre and Reynolds average of the static temperature to differ. Another consequence is seen in the change of shape of the Reynolds shear stress profile $\rho u'' w''$, the stress extremum
moving up to the location of the maximal density fluctuations. Thus some compressible turbulence statistics no longer follow the incompressible pattern and the validity of Morkovin’s hypothesis is restricted.

Further, the total temperature fluctuations cannot be neglected (not even for $M_\infty = 3$), which invalidates many of the assumptions made in deriving the strong Reynolds analogy (SRA). Thus, the perfect anti-correlation between $u''$ and $T''$ ($R_{u''T''} = -1$) predicted by the SRA is not realized. Nevertheless, some alternative or extended formulations perform reasonably well. Modeling approaches which are so far mainly based on homogeneous (shear) turbulence DNS data fail to correctly predict compressibility effects in boundary layers.

The present work has explored the still partly unknown world of the turbulent boundary layers in the high supersonic regime, and brought remarkable results. With the experience gathered in the meantime, some suggestions for improvement and directions for future work can be given. It would be interesting to implement the items described in section 8.5 (pressure formulation, zero mean spanwise flow) in order to see how large the benefits could be. With more CPU time available (or a yet faster computer) one could use more samples and thus improve the turbulence statistics. Performing more spatial steps would allow to study better the convergence of the solution towards accepted reference flows, particularly when the initial conditions are approximate or of poor quality. We observed that even in this case the ETDNS method makes the flow evolve towards a “physical” solution within a few spatial steps.

As already mentioned, direct numerical simulations are limited today to relatively low Reynolds numbers, although for the first time experimental Reynolds numbers ($Re_\theta$) were reached with the present high-supersonic turbulent boundary-layer DNS. The possibility to increase the Reynolds numbers of the DNS by orders of magnitude would give the opportunity on the one hand to investigate more efficiently the influence of this parameter and on the other hand to tackle problems of industrial relevance. For this purpose, one could wait until the supercomputers have reached the necessary speed and memory capacities. An attractive alternative is to employ the large-eddy simulation technique (LES), where some new and very promising subgrid-scale models are emerging, see e.g. [50, 4, 80].
Appendix A

Characteristic boundary conditions

The time-dependent characteristic boundary conditions used in the numerical algorithm at the upper domain boundary are formulated in the following way. The Navier-Stokes equations (2.2) can be written as

\[
\frac{\partial \mathbf{U}}{\partial t} = \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \frac{\partial \mathbf{H}}{\partial z} + \frac{\partial \mathbf{H}}{\partial z} + \mathbf{Z}_0 + \mathbf{Z}_1 + \mathbf{Z}_c \quad (A.1)
\]

where \( \mathbf{H} \) denotes the hyperbolic part and \( \mathbf{H} \) the parabolic part of the flux. The hyperbolic part can be expressed as

\[
\frac{\partial \mathbf{H}}{\partial z} = \frac{\partial \mathbf{U}}{\partial \mathbf{V}} \mathbf{S}_r \mathbf{A} \mathbf{S}_l \frac{\partial \mathbf{V}}{\partial z} \quad (A.2)
\]

where

\[
\mathbf{V} = \{\rho, u, v, w, p\} . \quad (A.3)
\]

\( \mathbf{S}_l \) and \( \mathbf{S}_r \) are the left and right eigenvector matrices and

\[
\frac{\partial \mathbf{U}}{\partial \mathbf{V}} \mathbf{S}_r = \begin{bmatrix}
1 & 0 & 0 & 1 & 1 \\
u & \rho & 0 & u & u \\
v & 0 & \rho & v & v \\
w & 0 & 0 & w - c & w + c \\
\frac{q^2}{2} & \rho u & \rho v & (\frac{q^2}{2} - cw + \frac{c^2}{\gamma - 1}) & (\frac{q^2}{2} + cw + \frac{c^2}{\gamma - 1})
\end{bmatrix} \quad (A.4)
\]

where \( q \) is the magnitude of the velocity vector (\( q^2 = u^2 + v^2 + w^2 \)).

The eigenvalues of the local flux Jacobian of the one-dimensional reduced hyperbolic system in \( z \) are the entries of

\[
\mathbf{A} = \text{Diag}\{\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5\} = -\text{Diag}\{w, w, w, w - c, w + c\} . \quad (A.5)
\]

They can be interpreted as follows: \( \lambda_2 \) and \( \lambda_3 \) are the velocities at which \( u \) and \( v \) are advected in the \( z \) direction, \( \lambda_1 \) is the convection velocity (wave-speed of entropy waves), \( \lambda_4 \) and \( \lambda_5 \) are the velocities of sound waves traveling
in negative and positive $z$ direction. The boundary condition is enforced by modifying the eigenvalues $\lambda_\nu$ of the diagonalized flux Jacobian $\Lambda$ to $\lambda_\nu^\circ$ in

$$
\Lambda^\circ S_t \frac{\partial V}{\partial z} = \begin{bmatrix}
\lambda_1^\circ \left( \frac{\partial \rho}{\partial z} - \frac{1}{c^2} \frac{\partial p}{\partial z} \right) \\
\lambda_2^\circ \frac{\partial u}{\partial z} \\
\lambda_3^\circ \frac{\partial v}{\partial z} \\
\lambda_4^\circ \left( -\frac{\rho}{2c} \frac{\partial w}{\partial z} + \frac{1}{2c^2} \frac{\partial p}{\partial z} \right) \\
\lambda_5^\circ \left( \frac{\rho}{2c} \frac{\partial w}{\partial z} + \frac{1}{2c^2} \frac{\partial p}{\partial z} \right)
\end{bmatrix}
$$

by setting

$$
\lambda_1^\circ = \lambda_2^\circ = \lambda_3^\circ = \begin{cases} 
-w & , \quad w \geq 0 \\
0 & , \quad w < 0
\end{cases}
$$

$$
\lambda_4^\circ = \begin{cases} 
-(w - c) & , \quad w - c \geq 0 \\
0 & , \quad w - c < 0
\end{cases}
$$

$$
\lambda_5^\circ = \begin{cases} 
-(w + c) & , \quad w + c \geq 0 \\
0 & , \quad w + c < 0
\end{cases}
$$

To summarize, the free-stream boundary conditions are enforced by

1. diagonalizing the reduced hyperbolic system
2. setting the eigenvalues along the incoming characteristics to zero
3. projecting forward in time.
Bibliography


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