Boundary Conditions for Spectral Simulations of Atmospheric Boundary Layers

by

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Abstract
An atmospheric boundary layer (ABL) is generally a very high Reynolds number boundary layer over a fully rough surface that is influenced by different external forces. Numerical simulations of ABLs are typically demanding, particularly due to the high Reynolds numbers. Large eddy simulation (LES) where the grid filtered Navier–Stokes equations are solved together with a turbulence model for the subgrid-scale motions is the most accurate and widely used technique to date for ABLs. However, high Reynolds numbers, filtered equations and rough surfaces do not support the simple no-slip boundary conditions together with a feasible grid resolution. A paramount part for the performance of an ABL LES simulation therefore lies in the quality of approximate wall boundary conditions, so called wall models.

The vast majority of LES codes used for ABL simulations rely on spatial discretization methods with low order finite difference approximations for the derivatives in the inhomogeneous wall normal direction. Furthermore, the wall boundary conditions are typically chosen in a mesh-dependent, non-local way, relying on the finite differences formulation.

In this thesis we focus on solving the ABL LES equations with a fully (pseudo) spectral Fourier–Chebyshev code. We present how wall boundary conditions can be formulated through Robin boundary conditions and how to implement these in the normal-velocity normal-vorticity formulation that we solve. A new idea of specifying boundary conditions directly in Fourier space where also the turbulence intensity statistics can be controlled is presented and verified. The present results show that the Robin-type formulation is effective at least in near-equilibrium boundary layers.

The code and boundary conditions were tested in both low and high Reynolds number (open and full) channel flows of neutral and stable stratification. Results were validated with both low to moderate Reynolds number DNS statistics as well as with the logarithmic law. Our results indicate great potential for both the the new boundary condition formulation and the specific code implementation. Further analysis of more complex flow situations will show whether the Robin-type formulation will give similarly good results.

Keywords: atmospheric boundary layers, boundary conditions, large-eddy simulation, spectral methods, wall model
Randvillkor för Spektrala Simuleringar av Atmosfäriska Gränsskikt

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Sammanfattning

Majoriteten av alla LES koder som används för ABL simuleringar är baserade på en lågordnings finita-differens diskretisering för derivatorna i den inhomogena väggnormalriktningen. Dessutom så är vägg-randvillkoren typiskt valda nätberoende och icke-lokala och direkt beroende av finita-differens diskretiseringen.


Nyckelord: atmosfäriska gränsskikt, large-eddy simulation, randvillkor, spektrala metoder, väggmodell
Preface

In this monograph I present the research from my first two and a half years as a PhD student at KTH mechanics.

The thesis concerns new ideas and implementation details of wall boundary conditions for atmospheric boundary layers in the Fourier–Chebyshev spectral code SIMSON developed and used at KTH mechanics since the 1990s.

The PhD project was founded by the Swedish research council (VR, Vetenskapsrådet) as a part of a larger project regarding fluid physics of complex wind farms. The simulations in this thesis were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at the High Performance Computing Center North (HPC2N).

December 2017, Stockholm

Erik Boström
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Chapter 1

Introduction

The atmospheric boundary layer (ABL) is the region of the atmosphere that is in direct contact with the surface of the Earth. The wind inside the ABL is generally turbulent and influenced by the shear stresses due to the rough surface, the rotation of the Earth and the buoyancy forces of temperature differences. Simulations of atmospheric boundary layer flows are of interest by meteorologists to understand the weather and climate but also by engineers to study the turbulent flows for wind-energy applications. Accurate turbulence simulations of ABLs with boundary conditions that can take into account the effects of the rough boundary are of paramount importance to study the complex flow physics inside and around wind farms.

Numerical computations of turbulent flows are generally complex and demanding. Turbulence is a highly non-linear and chaotic phenomenon that in a simulation must be captured by the discretized differential equations that are solved on a finite precision computer. The research problems one faces are typically a mix of physical, numerical and of computer-science characters. Physical in terms of understanding what to capture with the equations and the impact of necessary approximations, numerical in understanding the mathematical formulations and the influence of errors in the solution, and computer-science in the understanding how to actually solve the possible large scale systems on a (parallel) computer in an efficient way.

A turbulent flow includes a wide range of swirling motions called “eddies” that ranges from the size of the physical domain down to the size where their energy dissipate into heat due to viscosity. Furthermore, eddies of different sizes interact with each other. Hence in a simulation it becomes necessary to resolve all of them in order to accurately capture all the relevant physics of the flow. For the purpose of the work in this thesis we are interested in simulations of the wind in the atmospheric boundary layer, and particularly in flows around wind parks. For such types of flows the largest eddies covers the full height of the boundary layer and becomes approximately a kilometer in diameter; furthermore, the smallest scales are typically in size of millimeters. Thus, in order to accurately compute such flows with all the physical interactions between the scales we need a mesh that is very dense and a domain that is very large. A rough estimation of the number of grid points needed for such simulation is of order
\(O(10^{17})\). Add to that also the similar requirement in resolution for the discrete time-steps and the memory requirements. Unfortunately, such simulation is not feasible to do in a reasonable way at present time, even with help of the best supercomputers in the world. Solving the fluid dynamical equations in a direct way like this, where all scales are resolved, is called a “direct numerical simulation” (DNS). Such simulations can be done for \textit{e.g.}, small to moderate Reynolds numbers (\(Re = UL/\nu\), where \(U\) is a velocity scale, \(L\) a length scale and \(\nu\) the viscosity; see also §2.1.4.1). With an increased computer power such simulations have been frequently conducted over the last decades for higher and higher Reynolds numbers but are to date not even close to the Reynolds number of an atmospheric flow.

However, it is usually not necessary to solve for all the time and spatial scales appearing in a fluid flow problem for finding a practical solution of a problem at hand. Rather, there is an interest in fast simulation techniques where a quick results are in favor of high accuracy; this is often the case in industry or time-critical environments, such as \textit{e.g.} the weather forecast. Moreover, in the past when the computers were overall much weaker, approximations were needed to do the most simple flow simulations. Thus, much effort has been spent over the years to find approximations to the flow equations which include terms that approximate effects of the turbulence instead of resolving all the scales of it. The least expensive such approach is to decompose the flow variables, velocity \(u\) and pressure \(p\), into their mean and fluctuation parts \(u = \langle u \rangle + u'\) and \(p = \langle p \rangle + p'\), substitute these into the governing equations and approximate all terms that depend on the fluctuations \(u', p'\) in terms of mean quantities \(\langle u \rangle, \langle p \rangle\). This approach is called RANS (Reynolds Averaged Navier Stokes). Since the averaged flow is smooth in nature the resolution requirements becomes low, RANS equations can often be solved on a simple laptop. However RANS simulations are only accurate up to the accuracy of their (often empirical) approximations for the fluctuations. For more detailed studies of turbulent flows RANS is not feasible. A more detailed approach than RANS is large eddy simulation (LES) which focus on solving for the eddies that the grid can resolve and to approximate the effects of the small subgrid scale eddies. This also leads to a decomposition as for RANS into \(u = \bar{u} + u^{SGS}\) where \(\bar{u}\) is the resolved (filtered) part of the velocity, and \(u^{SGS}\) is the subgrid scale part. See more details in §2.2. In this thesis we mainly focus on LES.

In a fluid flow simulation there is always a question about boundary conditions. Appropriate boundary conditions are indeed a serious issue in most turbulent simulations. First of all there is the problem of open boundaries such as inflows and outflows. In a turbulent simulation the inflow cannot be chosen in an exact way and typically some constructed artificial turbulence is used. At an outflow boundary it gets even more problematic; here something close to an exact boundary condition is seldom available. Thus, the best one can hope for is to impose a boundary condition that is unphysical and does not affect the flow in the interior of the domain too much. One commonly talks
about non-reflecting boundary conditions when \textit{e.g.}, an advection equation
is imposed at the boundary, and/or damping zones which acts to damp out
the turbulence as it approaches the boundary, in this context. However, in
simulations over homogeneous directions where the statistical quantities are
of interest the inflow/outflow problems becomes eliminated using a periodic
domain. As long as the turbulent structures are not longer or wider than the
domain size the approximation has shown to yield very accurate time and space
statistics for the flow quantities (see Kim \textit{et al.} 1987). Such a periodic configu-
ration is employed in this thesis. Secondly, there is the problem of boundary
conditions on solid boundaries. This might at a first sight seem unproblematic
since the tangential flow velocity physically becomes zero at the boundary which
is called a “no-slip” boundary condition. For a DNS no-slip is also generally
correct. However, for approximated flow equations over a relatively coarse grid
the no-slip boundary conditions becomes questionable. Moreover, if the surface
include small roughness-elements that cannot be meshed the no-slip boundary
conditions become even less justified. This is typically the situation for an
atmospheric boundary layer LES. In order to capture the overall effects from
such surfaces in an effective way, approximate boundary conditions are typically
used. Appropriate boundary conditions for LES is a paramount part of this
thesis; see the extensive discussion in §3.

Highly accurate spectral methods have been used extensively for simulations
of turbulent flows since the ground-breaking series of papers by Steven Orszag;
(see \textit{e.g.} Orszag 1969). Generally speaking a spectral method is a numerical
method that seeks for an approximate solution to a partial differential equation
in form of a truncated series expansion of infinitely differentiable global basis
functions. Such a basis typically implies an exponential convergence rate.
Commonly used basis functions for spectral methods are the trigonometric
Fourier basis and Chebyshev or Legendre polynomials. Fourier methods are
simple to implement but restricted to periodic domains whereas Chebyshev
and Legendre polynomials can be used also for non-periodic problems. An
important ingredient of paramount importance in spectral methods for fluid
dynamical problems is the fast Fourier transform (FFT), that is often (but
not necessarily) used to treat non-linear terms. If a non-linear term is treated
with an explicit time-discretization, one can using FFT do differentiation in
spectral space (directly by multiplication for the Fourier method) and evaluate
products in physical space. With such a technique applied the method is
usually called a “pseudo-spectral” method. A popular spectral formulation
for three-dimensional flows over a domain with one inhomogeneous direction
(like a channel flow or an ABL) is to use Fourier series in the homogeneous
directions and Chebyshev polynomials over the inhomogeneous one. This leads
to a periodic box domain where the homogeneous directions are approximated
as periodic. Such a formulation is utilized in this thesis; see §4. The Chebyshev
basis is in this context usually chosen over the Legendre ones since the Chebyshev
polynomials can be transformed with FFT. For spectral methods not treating
the non-linear term pseudo-spectrally the Legendre polynomials are on the
other hand popular due to their rapid convergence and nice mathematical properties (for more information see e.g. Canuto et al. (1988)). For LES of ABLs the vast majority of existing codes employ (often second order but also fourth order) finite differences discretizations of the derivatives over the inhomogeneous wall normal direction. Such methods are simple to implement and boundary conditions can be chosen locally. The accuracy to resolve steep gradients is however inferior to spectral methods, in particular if the resolution is low (which is also often the case), and both numerical dissipation and dispersion will possible be present in the solution. As mentioned, in this thesis on the other hand we use a Chebyshev method in the inhomogeneous direction, similar to many DNS studies of channel flows (e.g., Kim et al. 1987; Moser et al. 1999). However, in our case we need to impose more complicated boundary conditions. The main differences between a Chebyshev and a finite differences (and also finite elements) approximation of a derivative at a grid point is that the finite differences method is local and uses only the neighboring grid values to approximate a derivative while the Chebyshev approximation is global in the sense that it uses values from points in the whole domain in its approximation. The global nature of the Chebyshev method leads to the exponential accuracy mentioned above. However, the global nature also makes the solution computed by the Chebyshev method at a given point dependent on the solution in all other points. Thus, the boundary conditions for a Chebyshev method cannot be imposed in a local way, as boundary conditions are imposed for finite differences methods. The global character also makes the Chebyshev method sensitive to local singularities which influences the solution in all points. The finite differences method is not as sensitive to local errors and discontinuous due to its local nature.

The main goal of the actual PhD project is to develop simulation tools based on spectral methods, to perform accurate turbulent simulations of atmospheric boundary layers for wind farm flows. The simulation tools should handle high Reynolds numbers, take surface roughness into account to approach flows over forests and include an active scalar dynamics to simulate stratified conditions representing day-time and night-time atmospheric conditions. Wind farms are to be included in the simulations by e.g. external body forces through the available actuator disc and line techniques. Available tools are necessarily further developed with spectral method frameworks in mind and should be computationally efficient to make it possible to solve large scale problems on supercomputers.

The main achievements of the work in this licentiate thesis are the following: (i) New boundary condition ideas for LES of atmospheric boundary layers using partial slip (Robin) boundary conditions that are based on both the logarithmic law and the attached eddy hypothesis have been proposed and tested. The tests shown are very promising, and potentially allow a mathematically more rigorous formulation of the employed wall models in atmospheric boundary layer
(ii) A new boundary condition implementation for our Fourier–Chebyshev code in which either Dirichlet, Neumann or Robin conditions can be imposed on the vertical boundaries has been developed. This new version of the code performs equally fast as the old version, but is much more flexible.

The thesis is organized as follows. In Chapter 2, the governing equations are presented. The Navier–Stokes equations in dimensional and dimensionless forms are presented, the application of the Boussinesq approximation for an active scalar is discussed and furthermore the filtered equations for large-eddy simulation are derived together with a short review of the eddy-viscosity approximation and the Smagorinsky model for both a neutral and stratified conditions. Chapter 3 concerns wall boundary conditions and wall modeling for large-eddy simulation. Here we review the typical mathematical boundary conditions that are commonly used and we summarize different wall modeling alternatives that are used for LES but also in other similar fluid dynamical areas where wall modeling is applied. Finally we present new ideas of wall boundary conditions for atmospheric boundary layers that can be used also for a Chebyshev method. In Chapter 4, the numerical method is presented which includes the derivation of the normal-velocity normal-vorticity equations and the discretization and solution process using the Chebyshev-tau method. The new boundary condition implementation in the code is explained in detail. Chapter 5 concerns numerical results that were obtained with the new version of the code and boundary condition. Canonical flow cases with one inhomogeneous direction are presented, i.e., open and full channel flow for both low and high Reynolds numbers. The chapter is closed by a short preliminary study of stably stratified simulations.
Chapter 2

Governing equations

In this introductory chapter we present the fluid dynamical equations that we later discretize and solve. In section 2.1 we consider the fundamental Navier–Stokes equations and apply the Boussinesq approximation. The equations are presented in both dimensional and non-dimensional forms. In section 2.2 we further consider the space-filtered versions of the equations and present the basics of large-eddy simulation (LES) using eddy-viscosity and diffusivity models.

2.1. Navier–Stokes equations

The equations governing the motion of a fluid are known as the Navier–Stokes equations, proposed for the first time by Claude-Louis Navier in 1822 and finally justified as a continuum model by George Gabriel Stokes in 1845. For a velocity vector $\mathbf{u}(\mathbf{x}, t) \in \mathbb{R}^3$ and a pressure scalar $p(\mathbf{x}, t) \in \mathbb{R}$ defined over space $\mathbf{x} \in \mathbb{R}^3$ and time $t \geq 0$ these are given by

$$\rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) + \nabla p - \nabla \cdot \left[ 2\mu \nabla^s \mathbf{u} + \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbb{I} \right] = \rho \mathbf{g}$$  \hspace{1cm} (2.1a)
$$\frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho + \rho (\nabla \cdot \mathbf{u}) = 0$$  \hspace{1cm} (2.1b)

where $\rho(\mathbf{x})$ is a scalar density field, $\mu(\mathbf{x})$ is the kinematic viscosity of the fluid, $\mathbb{I}$ a $3 \times 3$ identity matrix, $\nabla := (\partial_{x_1}, \partial_{x_2}, \partial_{x_3})^\top$ the gradient operator and $\mathbf{g} := (0, 0, g)^\top$ the constant acceleration due to gravity. Here we also introduced the short hand notation $\nabla^s \mathbf{u} := (\nabla \mathbf{u} + (\nabla \mathbf{u})^\top)/2$ for the symmetric part of the gradient tensor $\nabla \mathbf{u}$ or the so called strain-rate tensor.

Equation (2.1a) models the conservation of momentum or the point-wise representation of Newton’s second law of motion (force = mass×acceleration). Equation (2.1b) models the conservation of mass. The derivation of the Navier–Stokes equations can be found in any textbook on fluid dynamics and turbulence; see e.g. Batchelor (1967) or Tennekes & Lumley (1972).

Equations (2.1a)–(2.1b) are the general compressible form of the Navier–Stokes equations. Through the rest of this thesis we will only consider the simplified incompressible version. However, the compressible form is a necessary starting point in the understanding of the Boussinesq approximation which
we now present. The Boussinesq approximation makes it possible to use the incompressible formulation for a slightly compressible fluid flow.

2.1.1. The Boussinesq approximation

Let us decompose the density vector $\rho$ into its mean $\rho_0$ and fluctuating part $\rho'$ such that $\rho = \rho_0 + \rho'$. The Boussinesq approximation states that if $\rho' \ll \rho_0$ then all density fluctuations can be negligible except when they appear in the gravity term $\rho g$. Except for this term the equations therefore simplify to these used for an incompressible fluid:

$$\rho_0 \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) + \nabla p - \nabla \cdot [2\mu \nabla^s \mathbf{u}] = (\rho_0 + \rho')\mathbf{g},$$

$$\nabla \cdot \mathbf{u} = 0.$$  

The buoyancy term $(\rho_0 + \rho')\mathbf{g}$ can now, by assuming that the density has a linear dependency on temperature, be rewritten in terms of temperature (in the atmospheric boundary layer typically a potential temperature$^1$) $\theta$ by introducing a thermal expansion coefficient $\beta_\theta$, such that

$$(\rho_0 + \rho')\mathbf{g} = \rho_0\mathbf{g} - \rho_0\beta_\theta(\theta - \theta_0)\mathbf{g}.$$  

Here, $\rho_0\mathbf{g}$ becomes a constant value and can be moved into the pressure gradient to form a modified pressure: $p - \rho_0 g h \rightarrow p$ where $h$ is a height. Moreover, if the viscosity $\mu$ is assumed constant, i.e., $\mu = \mu_0$, then (2.2) can be rewritten as

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{1}{\rho_0} \nabla p - \nu_0 \Delta \mathbf{u} = \frac{\theta - \theta_0}{\theta_0} \mathbf{g},$$

$$\nabla \cdot \mathbf{u} = 0,$$  

where $\Delta := \nabla \cdot \nabla = \sum_{i=1}^3 \partial_i \partial_i$ is the linear Laplacian operator, and $\nu_0 = \mu_0 / \rho_0$ the constant kinematic viscosity. Here also an ideal gas was assumed, yielding $\beta_\theta = 1/\theta_0$. Note that, as $\nu_0$ is constant the incompressibility constraint implies

$$\nabla \cdot [2\nu_0 \nabla^s \mathbf{u}] = \nu_0 \partial_j (\partial_i x_j + \partial_j x_i) = \nu_0 (\partial_i (\partial_j x_j) + \partial_j x_i) = \nu_0 \Delta \mathbf{u}.$$  

2.1.2. Alternative forms of the nonlinear term

For an incompressible fluid the nonlinear advection term $\mathbf{u} \cdot \nabla \mathbf{u}$ can be written in different equivalent forms due to the incompressibility constraint $\nabla \cdot \mathbf{u} = 0$, e.g.,

$$\mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) = \omega \times \mathbf{u} + \frac{1}{2} \nabla (\mathbf{u} \cdot \mathbf{u}).$$  

where $\omega = \nabla \times \mathbf{u}$ is a vorticity vector. Here, the term leftmost is called the convective form, the one in the middle the divergence form and the one to the right is the so called rotational form. In numerical discretizations these are not necessary equal and the choice of which one to base the discretization on

$^1$A potential temperature $\theta$ is a scaled temperature such that under neutral conditions $\theta$ is constant with height, under stable conditions it increases with height, and under unstable conditions it decreases with height.
becomes important for the numerical properties of the discrete solution. For the spectral discretization we use the rotation form is the choice; see §4.

2.1.3. Scalar equation

The transport of a scalar quantity (such as temperature) \( \theta(x,t) \) within a flow field is governed by an advection-diffusion equation

\[
\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = \kappa_0 \Delta \theta
\]

(2.6)

where the constant \( \kappa_0 \) is a diffusion constant, and the velocity vector \( \mathbf{u} \) links (2.6) together with the momentum equation (2.4a). If the momentum equation (2.4a) is assumed to be unaffected by the scalar dynamics the scalar is called passive and there is a one-way coupling (the scalar equation depends on the velocity field but not the other way around). In reality however, like in the atmosphere, there is a two-way coupling due to the buoyancy term in (2.4a) and the scalar is then called active.

2.1.4. Non-dimensional forms and non-dimensional numbers

Similarity analysis, dimensional analysis and non-dimensionalization make it possible to compare flows of different fluids, velocities, temperatures, and/or length scales. The flow equations can be normalized by scales that characterize the flow of study to form equations that include universal, non-dimensional numbers.

Different non-dimensional numbers and their corresponding equations are derived below.

2.1.4.1. Reynolds number

Let \( V \) define a characteristic velocity scale (for a wall bounded flow e.g. the free-stream velocity) and \( L \) a characteristic length scale (e.g. the boundary layer height) of a particular flow. We here consider the incompressible Navier–Stokes equations with a general forcing function, i.e. equations (2.4) with \( f \) instead of \((\theta - \theta_0)g/\theta_0\). Multiplying (2.4a) and (2.4b) with \( L/V^2 \) we obtain the following non-dimensional formulation

\[
\left( \frac{\partial}{\partial t} \right)^* \mathbf{u}^* + \mathbf{u}^* \cdot \nabla^* \mathbf{u}^* + \frac{1}{\rho_0} \nabla^* p^* - \frac{1}{Re} \Delta^* \mathbf{u}^* = f^* \\
\nabla^* \cdot \mathbf{u}^* = 0
\]

(2.7a)

(2.7b)

where \((\partial/\partial t)^* := (L/V)(\partial/\partial t)\), \( \mathbf{u}^* := \mathbf{u}/V \), \( \nabla^* := L \nabla \), \( p^* := p/V^2 \), \( f^* := fL/V^2 \) and

\[
Re := \frac{VL}{\nu_0} = \frac{\text{inertial forces}}{\text{viscous forces}} = \frac{\text{intensity of the nonlinear effect}}{\text{intensity of the viscous linear effect}}
\]

(2.8)

is the non-dimensional Reynolds number. Note here that (2.4) and (2.7) are similar except for the viscous diffusive term where \( \nu_0 \) is now replaced by \( Re^{-1} \).
Mathematically, the Reynolds number controls the balance between the nonlinear advection term $\mathbf{u} \cdot \nabla \mathbf{u}$ and the linear diffusion term $\text{Re}^{-1} \Delta \mathbf{u}$; the larger the Reynolds number is, the more dominant the nonlinear effects become. As a consequence, flows at large Reynolds number may transition to turbulence easier than low Reynolds number flows and may contain much more complex dynamics.

For a turbulent flow the Reynolds number characterizes the size of the smallest turbulent eddies. As the Reynolds number increases these decrease in size while the largest eddies are still of the same size. Thus, the higher the Reynolds number is the wider the range of scales in the flow will be.

2.1.4.2. Prandtl number

Non-dimensionalization of the scalar (temperature) equation proceeds in a similar manner as for (2.7). Multiplying the scalar equation (2.6) with $L/(V\Theta)$ where $\Theta$ is a characteristic scalar scale, results in

$$
\left(\frac{\partial}{\partial t}\right)^* \theta^* + \mathbf{u}^* \cdot \nabla^* \theta^* = \frac{1}{\text{RePr}} \Delta^* \theta^*.
$$

(2.9)

where $\theta^* := \theta/\Theta$, $(\partial/\partial t)^*$ and $\nabla^*$ become similar as in (2.7). In (2.9)

$$
\text{Pr} := \frac{\nu_0}{\gamma_0} = \frac{\text{viscous diffusion rate}}{\text{thermal diffusion rate}}
$$

(2.10)

is the non-dimensional Prandtl number. Thus, a low $\text{Pr}$ indicates a flow where the thermal diffusion effects are dominant over the viscous diffusion effects and for a high $\text{Pr}$ the viscous effects dominate the thermal ones. The Prandtl number is directly dependent on the fluid, for air $\text{Pr} \approx 0.71$.

2.1.4.3. Richardson number

Consider again the non-dimensionalization of equation (4.1), but now including the buoyancy term. For the Boussinesq approximation we then get

$$
\mathbf{f}^* = \mathbf{f} \frac{L}{V^2} = -g\left(\frac{\theta - \theta_0}{\theta_0}\right) \frac{L}{V^2} \mathbf{e}_3 = \text{Ri} \theta^* \mathbf{e}_3
$$

(2.11)

where $\theta^* := (\theta - \theta_0)/(\theta_{\text{ref}} - \theta_0)$ (thus, here $\Theta = \theta_{\text{ref}} - \theta_0$) and

$$
\text{Ri} := \frac{g(\theta_{\text{ref}} - \theta_0)L}{\theta_0 V^2} = \frac{\text{buoyancy forces}}{\text{shear forces}}
$$

(2.12)

is the non-dimensional Richardson number. Typically, in a boundary layer $\text{Ri} < 0$ indicates unstable, $\text{Ri} = 0$ neutral, and $\text{Ri} > 0$ stable stratification. Other more complicated space dependent forms of Richardson numbers are also available, such as the “gradient Richardson number” or the “flux Richardson number”. These can be used characterize e.g. the local stability of a flow. See Garratt (1992) for more information. A gradient Richardson number will also appear in the modified Smagorinsky model presented in §2.2.5.
2. Large-eddy simulation

Solving the flow equations numerically on a coarse mesh the effects of the unresolved eddies are lost. This leads to physical errors since the unresolved eddies interact with the larger resolved ones; the equations that are solved are simply not the correct ones for the specific situation.

The aim of large-eddy simulation (LES) is to find new equations of motion that can be discretized on a coarse mesh and that capture the resolved turbulence accurately. Since small eddies are known to be more isotropic in nature than the large ones simple isotropic modeling assumptions are often used to model their effect. This is different from e.g. RANS where also the dynamics of the large eddies must be approximated, which requires typically much more complicated modeling approximations.

2.2.1. Space-filtered equations of motion

The equations of motion for LES can be obtained by applying a spatial convolution filter to the Navier–Stokes equations. Let \( \delta \) define a filter-width with a corresponding filter kernel \( g_\delta(x) \). Typically the filter-width is linked to the grid spacing of the mesh, but it can also be defined explicitly. For the Fourier–Chebyshev code the filter becomes implicitly of sharp-spectral type due to truncation in Fourier Space (see §4.2). Applying the filter to the velocity, pressure and temperature variables we define:

\[
\bar{u}(x,t) := (g_\delta * u)(x,t), \quad \bar{p}(x,t) := (g_\delta * p)(x,t), \quad \bar{\theta}(x,t) := (g_\delta * \theta)(x,t).
\]

Furthermore applying the filter to the incompressible Navier–Stokes equations we get

\[
\begin{align*}
g_\delta \left( \frac{\partial \bar{u}}{\partial t} + \nabla \cdot (\bar{u} \otimes \bar{u}) + \frac{1}{\rho_0} \nabla \bar{p} - \nu_0 \Delta \bar{u} - \frac{\theta - \theta_0}{\theta_0} g \right) &= 0, \\
g_\delta * (\nabla \cdot \bar{u}) &= 0, \\
g_\delta \left( \frac{\partial \bar{\theta}}{\partial t} + \nabla \cdot (\bar{u} \bar{\theta}) - \kappa_0 \Delta \bar{\theta} \right) &= 0,
\end{align*}
\]

where the nonlinear terms are written in the divergence form (for convenience as we will see soon). Assuming that the filter commutes with time and space derivatives it then follows that

\[
\begin{align*}
\frac{\partial \bar{u}}{\partial t} + \nabla \cdot (\bar{u} \otimes \bar{u}) + \frac{1}{\rho_0} \nabla \bar{p} - \nu_0 \Delta \bar{u} + \nabla \cdot T_u(u) &= \bar{\theta} - \theta_0 \frac{g}{\theta_0} \\
\nabla \cdot \bar{u} &= 0, \\
\frac{\partial \bar{\theta}}{\partial t} + \nabla \cdot (\bar{u} \bar{\theta}) - \kappa_0 \Delta \bar{\theta} + \nabla \cdot T_\theta(u, \theta) &= 0,
\end{align*}
\]

where

\[
T_u(u) := \bar{u} \otimes u \quad \text{and} \quad -\bar{u} \otimes \bar{u} \quad T_\theta(u, \theta) := \bar{u} \bar{\theta} - \bar{\bar{u}} \bar{\theta}
\]

are subgrid scale (SGS) fluxes.
2.2. Large-eddy simulation

**Remark 2.1.** Assuming that the filter commutes with space derivatives on a bounded domain (and even worse, if a non-uniform grid spacing is utilized) is not generally correct. A so called “commutator-error” will be introduced; see e.g. Ghosal & Moin (1995). However this fact is usually ignored in the derivation of the space-filtered equations.

The divergence terms $\nabla \cdot T_u$ and $\nabla \cdot T_\theta$ are the only differences between the standard and the space-filtered equations. They can be interpreted to include all the effects of the SGS motions.

However, $T_u(u)$ and $T_\theta(u, \theta)$ depend on unfiltered quantities, hence (2.13a) and (2.13c) are not closed. In order to solve (2.13) one need to rewrite $T_u(u)$ and $T_\theta(u, \theta)$ in terms of filtered quantities. This is however impossible to do in an exact way; for more information see e.g. Sagaut (2006) or Geurts (2004). Typically these terms are instead modeled.

### 2.2.2. Eddy-viscosity/diffusivity approximations

Usually in atmospheric boundary layer simulations so called eddy-viscosity and eddy-diffusivity models are used to close $T_u(u)$ and $T_\theta(u, \theta)$.

An eddy-viscosity model assumes that the SGS momentum flux tensor $T_u(u)$ is aligned to the resolved strain-rate tensor $\nabla^s \bar{u}$. It approximates the deviatoric part of $T_u(u)$ as follows

$$T_u^d(u) := T_u(u) - \frac{1}{3} \text{trace}(T_u(u)) \mathbb{I} \approx -2 \nu_t(x, t) \nabla^s \bar{u} \quad (2.15)$$

where $\nu_t(x, t)$ is the so called eddy-viscosity. The trace part of $T_u$, i.e., the normal part, can furthermore be moved into a modified pressure

$$\frac{1}{\rho_0} \nabla \bar{\rho} - \nabla \cdot \left[ \frac{1}{3} \text{trace}(T_u(u)) \mathbb{I} \right] = \nabla \left( \frac{1}{\rho_0} \bar{\rho} - \frac{1}{3} \text{trace}(T_u(u)) \right) \longrightarrow \nabla \bar{p}. \quad (2.16)$$

Similarly to an eddy-viscosity model the eddy-diffusivity model approximates the SGS temperature flux $T_\theta(u, \theta)$ by aligning it to the resolved temperature gradient $\nabla \bar{\theta}$:

$$T_\theta(u, \theta) \approx -\kappa_t(x, t) \nabla \bar{\theta}. \quad (2.17)$$

Using the eddy-viscosity and eddy diffusivity models, the space-filtered equations of motion (2.13a)–(2.13c) can be written as

$$\frac{\partial \bar{u}}{\partial t} + \nabla \cdot (\bar{u} \otimes \bar{u}) + \nabla \bar{p} - \nabla \cdot [\nu_0 + \nu_t(x, t)] \nabla^s \bar{u} = \frac{\bar{\theta} - \theta_0}{\theta_0} \mathbf{g}, \quad (2.18a)$$

$$\nabla \cdot \bar{u} = 0 \quad (2.18b)$$

$$\frac{\partial \bar{\theta}}{\partial t} + \nabla \cdot (\bar{u} \bar{\theta}) - \nabla \cdot [\kappa_0 + \kappa_t(x, t)] \nabla \bar{\theta} = 0, \quad (2.18c)$$

Thus, instead of a constant viscosity $\nu_0$ and a constant diffusivity $\kappa_0$ we now have a non-constant total viscosity $\nu_0 + \nu_t(x, t)$ and a non-constant total diffusivity $\kappa_0 + \kappa_t(x, t)$.
Equations (2.18a)–(2.18c) may also be written in non-dimensional form to yield expressions in terms of the non-dimensional numbers derived in §2.1.4. These are given by

\[
\frac{\partial \bar{u}}{\partial t} + \nabla \cdot (\bar{u} \otimes \bar{u}) + \nabla \bar{p} - \nabla \cdot \left[ \frac{1}{Re} + \nu_t(x, t) \right] \nabla \bar{u} = \text{Ri} \bar{\theta} e_3, 
\]
\[
\nabla \cdot \bar{u} = 0 \quad \text{(2.19b)}
\]
\[
\frac{\partial \bar{\theta}}{\partial t} + \nabla \cdot (\bar{u} \bar{\theta}) - \nabla \cdot \left[ \frac{1}{RePr} + \kappa_t(x, t) \right] \nabla \bar{\theta} = 0. \quad \text{(2.19c)}
\]

Here the star superscripts indicating non-dimensional quantities were dropped for the sake of simplicity.

**Remark 2.2.** When models are applied to approximate the SGS fluxes the solution sought is not \((\bar{u}, \bar{p}, \bar{\theta})\) of (2.13a)–(2.13c) but rather approximations to these quantities since we do not solve the same equations. However, for convenience we stick to the same notation also in (2.18a)–(2.19c).

It is important to stress the importance of the space and time dependency of \(\nu_t\) and \(\kappa_t\). The simplest choice to model \(\nu_t\) (or \(\kappa_t\)) is with a constant value. But if \(\nu_t\) (or \(\kappa_t\)) is constant the resulting filtered equations become similar to the original Navier–Stokes equations with a modified Reynolds number. Thus, a constant choice of \(\nu_t\) does nothing more than adding/removing dissipation to all resolved scales of the turbulent flow. However, what one wants is to add dissipation to the scales where the extra dissipation is needed which is mainly at the smallest resolved eddies.

The LES modeling problem has now turned into approximating the eddy viscosity and eddy diffusivity coefficients \(\nu_t(x, t)\) and \(\kappa_t(x, t)\). These both have dimensional units m²/s. By dimensional analysis these may therefore be written proportional to a product of a characteristic velocity scale \(V_{SGS}\) and a characteristic length scale \(L_{SGS}\) whose represent the velocity and size of the largest sub-filter scale eddies. Appropriate modeling of the eddy viscosity/diffusivity is therefore in finding approximations to \(V_{SGS}\) and \(L_{SGS}\).

### 2.2.3. The SGS Prandtl number

Recall, the Prandtl number was in §2.1.4.2 defined as the ratio of the viscosity and the diffusivity, i.e., \(Pr = \nu_0/\kappa_0\). Likewise to this molecular Prandtl number, a SGS Prandtl number can be defined as the ratio of the eddy-viscosity and the eddy-diffusivity:

\[
Pr_{SGS} := \frac{\nu_t(x, t)}{\kappa_t(x, t)} = \frac{\text{local viscous SGS diffusion rate}}{\text{local thermal SGS diffusion rate}}. \quad \text{(2.20)}
\]

In the literature the most common choice is to fix this Prandtl number to 0.6; see e.g. Sagaut (2006). Specifying the SGS Prandtl number like this the SGS diffusivity can be obtained as follows

\[
\kappa_t(x, t) = \frac{\nu_t(x, t)}{Pr_{SGS}} \approx \frac{\nu_t(x, t)}{0.6}. \quad \text{(2.21)}
\]
Thus, assuming a constant SGS Prandtl number we only need to find a model for \( \nu_t \). More complicated methods to determine both space and time varying \( \text{Pr}_{SGS} \) and \( \kappa_t \) are available, such as applying dynamic procedures. However for the scope of this thesis we keep the modeling as simple as possible and simply stay with \( \text{Pr}_{SGS} = 0.6 \).

### 2.2.4. The Smagorinsky model

The most commonly used SGS model for the eddy-viscosity is no doubt the Smagorinsky model. The Smagorinsky model is named after the meteorologist Joseph Smagorinsky and was first presented in his 1963 paper “General Circulation Experiments with the Primitive Equations”. However, a similar model had already been studied by von Neumann & Richtmyer (1950) as an artificial viscosity correction for compressible flows with shocks. For an extensive review of the history of the Smagorinsky model written by Smagorinsky himself see chapter 1 in Galperin & Orszag (1993).

The Smagorinsky model is a nonlinear eddy-viscosity model that is analogous to the Prandtl’s mixing length model in statistical modeling. In the Smagorinsky model the length scale \( L_{SGS} \) and the velocity scale \( V_{SGS} \) are both pre-specified. The length scale \( L_{SGS} \) is usually taken proportional to the grid spacing \( L_{SGS} \sim \delta \) and the velocity scale \( V_{SGS} \) is expressed in terms of the resolved strain rate tensor, \( V_{SGS} \sim \delta |\nabla^s \bar{u}| \) where \( |\nabla^s \bar{u}| := \sqrt{2(\nabla^s \bar{u} : \nabla^s \bar{u})} \). The Smagorinsky model may therefore be expressed as

\[
\nu_t(x,t) = (C_S \delta_S)^2 |\nabla^s \bar{u}|, \tag{2.22}
\]

where \( C_S \) is a (possible non-constant and local in space and time) proportionality coefficient, called the “Smagorinsky coefficient” and where \( \delta_S \approx \delta \) is a “Smagorinsky filter-width”.

The reason we see a need in introducing a separate \( \delta_S \approx \delta \) is that it is an approximation that should not be mistaken as a direct effect of the grid on the simulation. Moreover, since we typically have a three dimensional domain and \( \delta_S \) is a scalar quantity it is not directly clear how to approximate it if the grid-spacing is not uniform. For an uniform grid in all directions the choice of \( \delta_S \) is simple. The filter width proposed in the first LES paper by Deardorff (1970) was to take \( \delta_S \) as the geometric mean

\[
\delta_S = (\delta_1 \delta_2 \delta_3)^{1/3}. \tag{2.23}
\]

where \( \delta_j, j = 1, 2, 3 \) are constant filter widths for all the three directions of the grid. If \( \delta_1 = \delta_2 = \delta_3 \) then this definition also equals to all the definitions presented below. One may e.g. take an arithmetic mean

\[
\delta_S = (\delta_1 + \delta_2 + \delta_2)/3, \tag{2.24}
\]

or the following construction

\[
\delta_S = \sqrt{(\delta_1^2 + \delta_2^2 + \delta_3^2)/3}, \tag{2.25}
\]
or simply the maximum value

\[ \delta_S = \max\{\delta_1, \delta_2, \delta_3\}. \] (2.26)

However, if the grid-spacings in the different directions deviate from each other all these definitions differ. It is not clear which one to pick. Say for instance that the resolution in one direction is very dense and the resolution in the other two directions are very coarse. Then the geometric mean gives a \( \delta_S \) that is very small and the other three definitions a \( \delta_S \) that is very large. Thus, the choice of \( \delta_S \) is important when doing simulations with the Smagorinsky model. The problem with defining it is however often forgotten. The choice of \( \delta_S \) is indeed as important for the overall performance as the choice of the \( C_S \) coefficient or the magnitude of the strain rate tensor \( |\nabla^s \bar{u}| \).

For the choice of the Smagorinsky coefficient \( C_S \) on the other hand, it is widely known that in homogeneous isotropic turbulence it can be derived as \( C_S \approx 0.17 \), due to the work in Lilly (1967) by using the Kolmogorov K41 theory (Kolmogorov 1941). However, this value has shown to be too high for most flows. A modification in the derivations of \( C_S \) were turned out for different shapes of grid elements by Scotti et al. (1993) and Meyers & Sagaut (2007). Lilly’s derivation does in fact assume in fact integration over a sphere in its derivation, but a spherical volume becomes larger than a typical rectangular or cubic mesh element, thus the 0.17 value could be corrected to approximately 0.13 assuming cubic mesh elements instead. However, for boundary layer flows also \( C_S = 0.13 \) is too high. The Smagorinsky model assumes an equilibrium between the turbulence production and dissipation. For a flow that is anisotropic in the small SGS scales it is not accurate. This would e.g. be explained by the fact that \( |\nabla^s \bar{u}| \) becomes larger for such flows than in the isotropic case, and that an easy way to correct for it is to chose \( C_S \) smaller than the isotropic value (note that the same effect can also be achieved with a change in \( \delta_S \)). A well known universal value for boundary layer flows is however \( C_S = 0.1 \) which was also used in Deardorff (1970).

More general than separating \( \delta_S \) and \( C_S \) is to model them as a whole. This does further remove the grid influence on the Smagorinsky model. Such modeling can for instance be applied through a wall damping function (or similar ideas) or e.g. through dynamical models (Germano et al. 1991). More detailed information about damping functions are presented in the wall modeling chapter §3.4. Regarding dynamical models we do not employ such for any of the results presented in §5; we have in this thesis only focused on simple Smagorinsky models. We do therefore not present any details of the dynamical models here. We should however stress that do not ignore their performance, they are known to provide the best overall performance. However, they are also expensive and require extensive averaging to yield numerically stable results. More information about the dynamical models can be found in the original paper Germano et al. (1991) or in the books Sagaut (2006) or Geurts (2004).
2.2.4.1. Derivation of the Smagorinsky model

The Smagorinsky model can be derived from the SGS turbulence kinetic energy equation assuming equilibrium between the SGS production and dissipation. Let \( k' := \frac{(\vec{u} \cdot \vec{u} - \bar{\vec{u}} \cdot \bar{\vec{u}})}{2} \) define the SGS kinetic energy. An evolution equation for \( k' \) can be derived from the filtered Navier–Stokes momentum equation (here with no buoyancy term) as

\[
D_t k' = -T_u^d : \nabla^s \bar{\vec{u}} - \epsilon' + \nabla \cdot [\text{spatial redistribution terms}],
\]

where \( D_t := \partial_t + \bar{\vec{u}} \cdot \nabla \) is the material derivative, \( \epsilon' := \nu_0 (\nabla u : \nabla u - \nabla \bar{\vec{u}} : \nabla \bar{\vec{u}}) \) the SGS dissipation and \( -T_u^d : \nabla^s \bar{\vec{u}} \) is the SGS production. In an equilibrium flow all terms except for the production and dissipation cancel and we are left with

\[
\epsilon' = -T_u^d : \nabla^s \bar{\vec{u}}.
\]

Using the eddy-viscosity approximation (2.15) we then get

\[
\epsilon' = 2 \nu_t (\nabla^s \bar{\vec{u}} : \nabla^s \bar{\vec{u}}) = \nu_t |\nabla^s \bar{\vec{u}}|^2.
\]

Dimensional analysis gives \( \nu_t \simeq C_1 L_{SGS} V_{SGS} \) and \( \epsilon' \simeq C_2 V_{SGS}^3 / L_{SGS} \). Substitute these into the equation above and eliminate \( V_{SGS} \) to obtain

\[
\nu_t = C L_{SGS}^2 |\nabla^s \bar{\vec{u}}|.
\]

from which the Smagorinsky model follows.

Remark 2.3. Near a solid wall the equilibrium assumption does not hold and the performance of the Smagorinsky model becomes poor. In order to use the Smagorinsky model in such area it becomes necessary to apply some local modifications to it. A common modification is to apply a wall-damping function; see §3.4.

2.2.5. The modified Smagorinsky model for the Boussinesq approximation

In case the Boussinesq approximation is applied to the incompressible Navier–Stokes equations and a buoyancy-term is added to the momentum equation the SGS kinetic energy equation changes. An extra production/destruction term appears that corresponds to the buoyancy. Thus, assuming equilibrium the Smagorinsky model in its original form is no longer an accurate approximation since it does not take the buoyancy effects into account. However, as was first presented by Eidson (1985), a modified Smagorinsky model can be derived which has the limit of the Smagorinsky model as the buoyancy force tend to zero. The modified Smagorinsky model can be stated as

\[
\nu_t = (C_S \delta_S)^2 |\nabla^s \bar{\vec{u}}| T(\bar{\vec{u}}, \bar{\theta}), \quad \text{with} \quad T(\bar{\vec{u}}, \bar{\theta}) := \sqrt{1 - \frac{\text{Ri}_{SGS}(\bar{\vec{u}}, \bar{\theta})}{\text{Pr}_{SGS}}},
\]

(2.27)

where

\[
\text{Ri}_{SGS}(\bar{\vec{u}}, \bar{\theta}) := \frac{g}{\theta_0} \frac{\partial \bar{\theta}}{\partial x_3} / |\nabla^s \bar{\vec{u}}|^2
\]

(2.28)
is a local SGS Richardson number (also called a gradient Richardson number; see Garratt (1992)), and $\Pr_{\text{SGS}} \approx 0.6$ the SGS Prandtl number.

### 2.2.5.1. Derivation of the modified Smagorinsky model.

The derivation of the modified Smagorinsky model follows the same steps as the derivation of the original Smagorinsky model. With the buoyancy term added to the momentum equations, the $k'$ equation yields the following equilibrium condition:

$$
\epsilon' = -T^d_u : \nabla^s \bar{u} - \frac{1}{\theta_0} \mathbf{g} \cdot \nabla \theta.
$$

(2.29)

Substitution of an eddy-viscosity model and an eddy-diffusivity model into (2.29) gives

$$
\epsilon' = \nu_t(x, t) |\nabla^s \bar{u}|^2 + \frac{1}{\theta_0} \mathbf{g} \cdot \kappa_t(x, t) \nabla \bar{\theta} = \nu_t(x, t) \left[ |\nabla^s \bar{u}|^2 + \frac{g}{\theta_0} \frac{\partial \bar{\theta}}{\partial x_3} \right].
$$

Now, dimensional analysis yields $\nu_t \simeq C_1 L_{\text{SGS}} V_{\text{SGS}}$ and $\epsilon' \simeq C_2 V_{\text{SGS}}^3 / L_{\text{SGS}}$, and (2.27) follows.

**Remark 2.4.** The modified Smagorinsky model on the form (2.27) becomes imaginary for $\text{Ri}_{\text{SGS}}(\bar{u}, \bar{\theta}) / \Pr_{\text{SGS}} > 1$. To guarantee that (2.27) becomes positive one may e.g. rewrite $T$ as

$$
T(\bar{u}, \bar{\theta}) = \sqrt{1 - \frac{\text{Ri}_{\text{SGS}}(\bar{u}, \bar{\theta})}{\Pr_{\text{SGS}}}}.
$$

Another alternative is to set $T(\bar{u}, \bar{\theta}) = 0$ if $\text{Ri}_{\text{SGS}}(\bar{u}, \bar{\theta}) / \Pr_{\text{SGS}} > 1$, i.e., apply a “clipping” strategy.
Wall boundary conditions and wall modeling

In this chapter we examine the problem of wall boundary conditions and discuss alternative wall modeling strategies for atmospheric boundary layer flows using Robin boundary conditions and matching functions.

The structure of the chapter is as follows. In section 3.1 physical boundary conditions for the Navier–Stokes equations are discussed. In section 3.2 we present a short review on wall boundary condition strategies that have been used for LES, and shortly also the boundary condition ideas in the area of superhydrophobic and flows over porous media where similar approaches are needed. In section 3.3 we present new ideas regarding wall modeling through partial slip boundary conditions for atmospheric boundary layer. These were subsequently also implemented in our Fourier–Chebyshev code. Finally in section 3.4 we review damping/matching function alternatives to be used together with wall boundary conditions for the Smagorinsky model.

3.1. Wall boundary conditions for the Navier–Stokes equations

Suppose we want to solve the incompressible Navier–Stokes equations over a bounded domain $\Omega$ with a boundary $\partial \Omega$ that contains a solid wall $\Gamma \subset \partial \Omega$.

If $\Gamma$ is perfectly smooth the no-slip boundary condition for the tangential quantities holds

$$u \cdot \hat{\tau}_j = 0, \quad j = 1, 2 \quad \text{on} \ \Gamma,$$  

(3.1)

where $\hat{\tau}_j$, $j = 1, 2$ are unit tangential vectors over the surface. Moreover it is clear that for a solid wall there are no vertical movement of the fluid at $\Gamma$, which implies the no-penetration boundary condition for the normal velocity

$$u \cdot \hat{n} = 0, \quad \text{on} \ \Gamma.$$  

(3.2)

where $\hat{n}$ is the unit normal vector to the surface.

In some situations the no-slip boundary condition must be relaxed. For instance, the Navier–Stokes equations can aside from the conservation laws be derived from the kinetic theory of gases by an averaging process. This was done by Maxwell (1879). In the continuum limit the tangential velocities satisfy a
3. Wall boundary conditions and wall modeling

**partial slip** boundary condition

\[
\beta_j \mathbf{u} \cdot \hat{\mathbf{r}}_j + \hat{\mathbf{n}} \cdot \sigma(\mathbf{u}, p) \cdot \hat{\mathbf{r}}_j = 0, \quad j = 1, 2, \quad \text{on } \Gamma,
\]

where \( \beta_j \) are effective *friction coefficients* for the specific situation that in Maxwell’s derivation were obtained having the magnitude

\[
\beta_j^{-1} = O(\text{mean free path of molecules}).
\]

In (3.3) the tensor \( \sigma(\mathbf{u}, p) := \text{Re}^{-1} \nabla \mathbf{u} - p \mathbf{I} \) is the Cauchy stress tensor. These boundary conditions generate a partial slip on \( \Gamma \) which can be interpreted as the averaged flow properties over all liquid molecules near the solid boundary. These boundary conditions were indeed first studied by Navier (1823) and are commonly called the *Navier slip* law. Navier proposed these boundary conditions with an argument that the tangential stress has to be continuous from the solid wall to the fluid. These are in a sense a generalization of the no-slip boundary conditions, which are obtained in the limits \( \beta_j \to \infty \). On the other hand, as \( \beta_j \to 0 \) free-slip boundary conditions are obtained.

Over smooth boundaries \( \beta_j \) becomes extremely large since \( O(\text{mean free path of molecules}) \) is very small, hence no-slip boundary conditions are justified. Physical slip on smooth surfaces does therefore mainly appear at nano-scales and for gases. However over boundaries where the mean effects of the surface need to be taken into account in an averaged sense, such as for rough or hydrophobic boundaries the Navier law can be an alternative choice to the no-slip boundary conditions as an effective approximate boundary conditions taking into account the surface effects (see *e.g.* Min & Kim 2004). The friction coefficients \( \beta_j \) become then modeling coefficients that must be specified a-priori. In this sense, (3.3) often used in practical applications as approximate boundary conditions (wall models) where \( \beta_j \) become effective modeling parameters that can be estimated from measurements or theory.

### 3.2. Wall boundary conditions for the filtered Navier–Stokes equations

We now discuss boundary conditions for the filtered velocities in LES. For simplicity we let the domain \( \Omega \) be rectangular with a solid wall \( \Gamma \subset \partial \Omega \) at \( x_3 = 0 \) and with tangential directions \( x_1 \) and \( x_2 \). Corresponding velocity quantities are \( \mathbf{u} = (u_1, u_2, u_3)^\top \).

Listed below are some arguments for using wall models in large-eddy simulation:

(i) *Resolution requirements.* Closest to a solid boundary in a turbulent flow there is a thin region where viscous forces dominates which is called the viscous sublayer that becomes thinner with an increase in Reynolds number (see §3.2.1). The vertical velocity gradient inside the viscous sublayer gets steeper and steeper as the region gets thinner. In order to resolve the viscous sublayer in a wall bounded flow we need at least a few grid points inside it. However, for high Reynolds numbers the resolution
requirements to resolve it becomes impractically high. Imposing a no-slip boundary condition with a too coarse resolution may lead to problems for several reasons. First, there is a serious loss in accuracy. The simulated gradient at the wall is likely to be severely underestimated as the viscous sublayer cannot be resolved properly. Secondly, an under-resolved vertical gradient may lead to numerical instability. This is especially evident in a spectral code where this situation is similar to a discontinuity which leads to oscillations in the polynomial representation of the solution.

(ii) **Boundary conditions must be specified for the filtered velocities.** Boundary conditions for the filtered velocities \( \bar{u} = g_\delta * u \) need not necessarily be the same as these for \( u \). For a turbulent flow we can only guarantee \( \bar{u}_j |_{\text{wall}} \to 0 \) for \( j = 1, 2 \) in the limit \( \delta \to 0 \), or physically correct, in the limit of the smallest turbulent scales. It is however often not possible to increase the grid spacing this much in practice, in particular not for a very high Reynolds number flow. This problem is illustrated in Figure 3.1, here illustrated for a filtered region around a point at the boundary for a turbulent boundary layer mean profile.

(iii) **Rough surfaces.** In reality, a surface is never fully smooth. Indeed, for an atmospheric boundary layer the surface is always expected to be fully rough (see e.g. Garratt 1992) which means that the height of the individual roughness elements at a surface can be expected to be always larger than the height of the viscous sublayer. Also in most situations roughness elements are very small, and the complex structure of them cannot be meshed. Instead, the effect of the roughness elements must be taken into account in an averaged sense. In this case the no-slip boundary conditions must be replaced by some effective boundary conditions.
3. Wall boundary conditions and wall modeling

3.2.1. Law of the wall

Before we proceed to more discussion about wall boundary conditions and wall modeling strategies we need to introduce the law-of-the-wall concept of a wall bounded flow. The law of the wall, and particularly the logarithmic law are widely used for wall modeling approximations and are crucial in order to understand the physics of a turbulent flow in the vicinity of a solid boundary.

The total stress of a wall bounded flow can be divided up into two parts:

(i) viscous stress: \( \nu_0 \partial_3 \langle u_j \rangle, j = 1, 2 \); and

(ii) turbulent stress (or Reynolds stress): \( \langle u'_j u'_3 \rangle, j = 1, 2 \),

where \( u'_j := u_j - \langle u_j \rangle \) defines the fluctuating part of the velocity. At a solid wall only the viscous stress is non-zero. This stress is called the wall-shear stress \( \tau_w \) and is defined over a horizontal flat wall as

\[
\tau_w := \rho_0 \nu_0 \frac{\partial U}{\partial x_3} \bigg|_{\text{wall}}, \quad U := \sqrt{\langle u_1^2 \rangle + \langle u_2^2 \rangle}.
\] (3.4)

Here \( U \) is simply defined as the mean horizontal velocity. From the wall shear stress an important velocity scale, the friction velocity \( u_\tau := \sqrt{\tau_w/\rho_0} \) is defined. Away from the wall the turbulent stress \( \langle u'_j u'_3 \rangle \) becomes more and more dominating. The mean velocity profile can be written as

\[
U^+ = f(x^+_3).
\] (3.5)

where \( f \) is called law of the wall. Here

\[
U^+ := \frac{U}{u_\tau} \quad \text{and} \quad x^+_3 := \frac{u_\tau x_3}{\nu},
\] (3.6)

de note so called wall units (or viscous units). Notice that \( x^+_3 \) indeed is a local Reynolds number. The Reynolds number determines a relation between inertial and viscous forces, thus \( x^+ \) is a measure of the relative importance of viscous and turbulent processes. By dimensional analysis and matching one can derive an expression for \( f \). One such is the Prandtl–Taylor law that states

\[
\begin{align*}
&f(x^+_3) = x^+_3, & 0 \leq x^+_3 \lesssim 5, \quad (3.7a) \\
&f(x^+_3) \neq x^+_3, \quad f(x^+_3) \neq \frac{1}{\kappa} \log(x^+_3) + B, & 5 \lesssim x^+_3 \lesssim 30, \quad (3.7b) \\
&f(x^+_3) = \frac{1}{\kappa} \log(x^+_3) + B, & x^+_3 \gtrsim 30, \quad x_3 \lesssim 0.3L_3. \quad (3.7c)
\end{align*}
\]

where \( L_3 \) is the dimensional height of the boundary layer, the constant \( \kappa \) is the von Kármán constant (typically around 0.4) and \( B \) a constant (around 5.2 for a smooth wall); see Pope (2001). When we refer to different regions through
3.2. Wall boundary conditions for the filtered Navier–Stokes equations

the thesis, we mean, according to Pope (2001) that

\[
\begin{align*}
\text{viscous sublayer} & \quad x_3^+ \lesssim 5; \\
\text{viscous wall region} & \quad x_3^+ \lesssim 50; \\
\text{outer layer} & \quad x_3^+ \gtrsim 50; \\
\text{inner layer} & \quad x_3 \lesssim 0.1L_3 \\
\text{buffer layer} & \quad 5 < x^+ \lesssim 30; \\
\text{log region} & \quad x_3^+ \gtrsim 30, \quad x_3 \lesssim 0.3L_3;
\end{align*}
\]

The law-of-the-wall in the logarithmic region can be rewritten for a flow over a fully rough \((h_r \gg \text{viscous sublayer})\) surface as

\[
U = \frac{U_\tau}{\kappa} \log(x_3/h_r), \quad x_3 \gg h_r, \quad (3.8)
\]

where \(h_r\) is the so called roughness height.

3.2.2. Conventional wall stress models for LES derived for staggered finite differences

Slip-type boundary conditions for LES have been used since the first LES papers by Deardorff (1970) and Schumann (1975) in the 1970s. These early LES papers were indeed the first serious attempts to simulate a smooth-wall channel flow before any DNS of such flows were conducted. The wall models they used where designed to eliminate viscous sublayer according to point (i) (however (ii) is also affected), they could not afford a resolution to resolve the steep vertical gradient. Both used a staggered grid setup in the vertical direction and second-order finite-differences discretizations of the vertical derivative. Deardorff suggested a model on the second derivatives of the velocities where he tried to include effects of fluctuations. His model was based on the logarithmic law \((3.7c)\) and therefore Reynolds number independent. Schumann proposed a model (see below) for the wall shear stress which could be imposed easily as a flux at the boundary in his finite volume code. The Schumann model has been further developed with several modifications. For a detailed description of all these different modifications; see Sagaut (2006) p. 323–353.

3.2.2.1. Schumann’s model

Let \(x = (x, y, z)^\top \in \Omega\) and \(u = (u, v, w)^\top\) where \(\Omega\) is here a box domain with \(x\) (\(u\)) the streamwise, \(y\) (\(v\)) the spanwise and \(z\) (\(w\)) the vertical directions (velocities). In a staggered grid setup let \(z = z_0 = 0\) be the location of a solid wall and \(z = z_{1/2}\) the first grid point above it. The horizontal quantities are solved at the half grid indices \((1/2, 3/2, \ldots)\), and the fluxes (derivatives) at the full indices \((0, 1, \ldots)\). A one-sided finite differences approximation of the instantaneous wall shear stress can now be written as follows in that framework

\[
\tau_{xx,1/2} = \nu_{tot} \frac{\partial u}{\partial z}_{1/2} \approx \nu_{tot} \frac{u(z_{1/2}) - u(0)}{z_{1/2}} = \nu_{tot} \frac{u_{1/2}}{z_{1/2}} \approx \tau_{xx,0}. \quad (3.9)
\]
where \( u(0) = 0 \) was applied. The approximation of the wall shear \( \tau_{xz,0} \) is here a simple extrapolation. A similar expression is obtained also for \( w \). The ensemble averaged wall shear stress can now be approximated as

\[
\langle \tau_{xz,0} \rangle = \nu_{\text{tot}} \left( \frac{u_{1/2}}{z_{1/2}} \right).
\]

(3.10)

Combining (3.9)–(3.10) it follows that

\[
\tau_{xz,0} = \frac{\langle \tau_{xz,0} \rangle}{u_{1/2}} u_{1/2}
\]

(3.11)

which simply states that \( \tau_{xz,0} \propto u_{1/2} \). In (3.11) the averaged wall shear stress \( \langle \tau_w \rangle = u_w^2 \) must be specified; it is known a-priori for the channel flow simulation by an applied constant pressure gradient. Furthermore the averaged velocity \( \langle u(z_1) \rangle \) must also be specified; it is approximated assuming the logarithmic law holds at \( z_{1/2} \).

For the vertical velocity Schumann used a no-penetration boundary condition. In three dimensions the boundary conditions can be stated as

\[
\begin{aligned}
\tau_{xz,0} &= \left( \frac{u_w^2}{\sqrt{\langle u_{1/2} \rangle^2 + \langle v_{1/2} \rangle^2}} \right) u_{1/2}, \\
\tau_{yz,0} &= \left( \frac{u_w^2}{\sqrt{\langle u_{1/2} \rangle^2 + \langle v_{1/2} \rangle^2}} \right) v_{1/2}, \\
w_0 &= 0.
\end{aligned}
\]

(3.12)

Note that, since \( w_0 = 0 \) it follows that \( u_0 w_0 = v_0 w_0 = 0 \) and \( \tau_{xz,0} \) and \( \tau_{yz,0} \) becomes the total fluxes at the boundary.

The Schumann model is seldom used nowadays. The interest in low accuracy approximations of wall-modeled channel flows that are simulated with finite differences approximations in the wall normal direction is rather low. As the computers have grown stronger, moderate Reynolds number DNSs of channel flows with a fully resolved inner regions are now standard and engineering flows are generally over non-homogeneous surfaces such as vehicles where pressure variations are present and the Schumann model does not apply. For atmospheric flows over a flat surface the Schumann model is still an alternative. However, here often an even simpler approach of directly impose the logarithmic law is instead applied (see below).

3.2.2.2. Moeng’s model

A commonly used wall model for LES of atmospheric boundary layers is similarly to the Schumann model to approximate the instantaneous fluxes, but instead of formulating a linear relationship between the stress and horizontal velocity to use the mean stress obtained from a logarithmic law assumption for the instantaneous quantities. We call it the Moeng model (Moeng 1984) but it is
3.2. Wall boundary conditions for the filtered Navier–Stokes equations

simply a wall function approach for RANS extended to LES; sometimes it is also referenced to Mason & Callen (1986).

Similar to the Schumann model, the fluxes are for the Moeng model applied to a discretization based on second order central finite differences in the wall normal direction. We therefore use the same notation.

Let here $h_r$ be an empirically defined roughness height. The logarithmic law for a rough wall then reads

$$\sqrt{(u_{1/2})^2 + (v_{1/2})^2} = \frac{u_{\tau}}{\kappa} \log \left( \frac{z_{1/2}}{h_r} \right),$$

which rewrites into

$$u_{\tau} = \left( \langle \tau_{w,xz} \rangle^2 + \langle \tau_{w,yz} \rangle^2 \right)^{1/4} = \left( \frac{\kappa}{\log(z_{1/2}/h_r)} \right) \sqrt{(u_{1/2})^2 + (v_{1/2})^2},$$

where $u_{\tau}^2 = \langle \tau_{w,xz} \rangle^2 + \langle \tau_{w,yz} \rangle^2$ is the mean wall shear stress expressed in terms of its horizontal quantities. Thus,

$$\sqrt{\langle \tau_{w,xz} \rangle^2 + \langle \tau_{w,yz} \rangle^2} = \left( \frac{\kappa}{\log(z_{1/2}/h_r)} \right)^2 \left( (u_{1/2})^2 + (v_{1/2})^2 \right).$$

If this is now split up into components in the directions of the instantaneous horizontal velocities and if we furthermore assume that the instantaneous stresses can be approximated by the averaged ones $\tau_{0,xz} \approx \langle \tau_{w,xz} \rangle$ and $\tau_{0,yz} \approx \langle \tau_{w,yz} \rangle$ then one obtains the following boundary conditions

$$\begin{cases} 
\tau_{0,xz} = \left( \frac{\kappa}{\log(z_{1/2}/h_r)} \right)^2 \sqrt{(u_{1/2})^2 + (v_{1/2})^2} u_{1/2}, \\
\tau_{0,yz} = \left( \frac{\kappa}{\log(z_{1/2}/h_r)} \right)^2 \sqrt{(u_{1/2})^2 + (v_{1/2})^2} v_{1/2}, \\
w_0 = 0,
\end{cases}$$

(3.13)

where also the no penetration condition for the vertical velocity was added. Note, that also the von Kármán constant $\kappa$ must be selected.

Several questions easily arise regarding the stress-type boundary conditions presented above. They are for instance both space and time dependent. What about well posedness? Can we be sure that they indeed converge to a reasonable result from a given initial condition? Can you be sure that they lead to a numerically stable result? They are derived in discrete form. What is the corresponding boundary conditions for the continuous problem?

None of the questions above seem to be answered clearly in the literature. For a staggered grid in the vertical direction and finite differences these stress boundary conditions may be easy to implement, but their performance is generally rather unclear. What the Moeng model assumes is that the log law holds at the first $u,v$ grid level in the staggered grid, then it feeds back a computed stress computed from the previous time step result down to the boundary. If the log law is not satisfied the approximation is not correct. Thus,
starting from a non-logarithmic initial condition it is not directly clear that
the should converge to something reasonable. These boundary conditions are
also grid dependent, they depend on the position of \( z_{1/2} \). The grid dependency
is problematic, as the grid resolution is increasing the term \( (\kappa/\log(z_{1/2}/h_r))^2 \)
will grow in size. In the limit \( z_1 \to h_r \) the boundary conditions blow up as
\( (\kappa/\log(z_{1/2}/h_r))^2 \to \infty \). Furthermore an error in the velocity at \( z_{1/2} \) will be
amplified as it is used in the boundary conditions.

In addition, approximating the instantaneous stress with a model based on
the averaged stress leads to obvious errors; for the Moeng model Bou-Zeid et al.
(2005) pointed out that the obtained stress indeed becomes overestimated. This
directly follows from \( \langle \tau_w \rangle = (\kappa/\log(z_1/z_0))^2 \langle u^2 \rangle \geq (\kappa/\log(z_1/z_0))^2 \langle u \rangle^2 \). Due
to this Bou-Zeid et al. proposed to use an extra filtering on the the instantaneous
velocities that the model is based on. They could see some improvements by
this procedure. However, adding extra filtering may damp fluctuations which
in the worst case may lead to relaminarization. In fact, the turbulence intensity
should be largest at the first grid level (if it is located in the log-layer), damping
the turbulence may give a better mean profile, but not a higher accuracy of the
turbulent field in general.

3.2.2.3. Zonal approaches and hybrid RANS/LES methods

The simple wall stress models presented above are derived for horizontally
homogeneous flows and cannot generally handle flow separation and pressure
variations. For large scale flat surface meteorological applications this is not
generally a big issue but for engineering problems they are not applicable.

So called zonal approaches (e.g. Balaras et al. 1996) do account for pressure
variations and separation by solving the boundary layer equations on an embed-
ded mesh between the first horizontal grid level and the wall (also here usually
described in a staggered finite differences framework). Shear stress boundary
conditions are directly computed from the upper boundary of the embedded
grid to the LES grid in each time step. Results for different types of zonal
approaches have been made and were compared on the backward-facing step
problem with moderate success; see Piomelli & Balaras (2002) and Piomelli
(2008).

RANS/LES hybrid approaches is another choice that is use two different
regions of the domain. One RANS region closest to the wall where the unsteady
RANS equations are solved. This region has a proper resolution to resolve the
near-wall region. The RANS layer has its own time and length scales. A lot
of effort has been made to make the matching between the RANS and LES
appropriate e.g. adding artificial fluctuations. The RANS/LES hybrids are
more accurate than the zonal approach but significantly more expensive.

However, for a fully rough atmospheric boundary layer where a viscous
sublayer does not exist these approaches cannot be applied directly. Another
drawback for these approaches is that they are computational costly. For
horizontally homogeneous flows they are not either better than more simple
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wall modeling alternatives (such as wall stress models); see the discussion in

3.2.3. Wall boundary conditions for LES using partial slip boundary conditions

Wall boundary conditions for LES based on the Navier boundary conditions
were proposed in the framework of finite elements by Galdi & Layton (2000).

Galdi & Layton suggest (according to point (ii) in §3.2 and Figure 3.1) that
even if the fluid satisfies the no-slip boundary condition on a solid boundary, the
LES approximation \( \bar{u} \) should satisfy partial slip and no penetration boundary
conditions (3.3). This assumes that the filter width does not decrease as a
boundary is approached and therefore has a non-zero value at the boundary.

Over a solid surface the Navier conditions (3.3) written for filtered velocities
becomes

\[
\bar{u} \cdot \hat{\tau}_j = 0, \quad \beta_j \bar{u} \cdot \hat{\tau}_j + \hat{n} \cdot \sigma_{\text{tot}}(\bar{u}, \bar{p}) \cdot \hat{\tau}_j, \quad j = 1, 2.
\]

(3.14)

where \( \sigma_{\text{tot}}(\bar{u}, \bar{p}) := 2[\nu + \nu_t(x, t)]\nabla^s \bar{u} - pI \) is the total stress tensor, including
the eddy viscosity. The friction coefficients \( \beta_j \) must be determined as these
become modeling parameters. From an a-priori known solution \( \bar{u} \) the \( \beta_j \)s can
be computed as

\[
\beta_j = -\frac{\hat{n} \cdot \sigma_{\text{tot}}(\bar{u}, \bar{p}) \cdot \hat{\tau}_j}{\bar{u} \cdot \hat{\tau}_j}, \quad j = 1, 2.
\]

(3.15)

As a follow up from the ideas of Galdi & Layton (2000), John et al. (2004)
derived different friction parameters for the filtered velocity. They used the
known 1/7th power law solution and included the analytic expression of the
Gaussian filter they used to obtain friction coefficients. They could show that
the friction parameters they obtained satisfied the limit \( \beta_j \to \infty \) as \( \delta \to 0 \n
\)
according to the limit of no-slip for the continuous problem. The boundary
conditions were imposed in a finite element code and they did run some test cases
on a two dimensional channel with a step of rather low Reynolds numbers. The
results were promising. John & Liakos (2006) furthermore did three dimensional
studies on the same test case where the step was simply extended in the spanwise
direction. They could see some shedding behind the step, but no extensive
validation was performed.

Another interesting study where slip boundary conditions for LES were
applied is that of Bose & Moin (2014). They derived a slip boundary condition
through the expression of an explicit inverse Helmholtz differential filter that they
applied to the Navier–Stokes equations. The corresponding friction coefficient
was obtained through a dynamic procedure (Germano et al. 1991) to directly
include the filtering effects. The Bose & Moin boundary condition recovers the
no-slip boundary conditions in the DNS limit. They could further accurately
predict the separation point on an airfoil using these boundary conditions. As
follow up studies, Bae et al. (2016) considered further these boundary conditions
in a channel flow setup, and Yang & Bose (2016) derived the friction parameter
from a logarithmic law in a similar way like we propose in §3.3.1 and tested the boundary conditions in a Re$_\tau = 2000$ channel flow. Results were in line with the results of a simple stress model.

3.2.3.1. A short review: slip boundary conditions as a wall model for flows over superhydrophobic surfaces and porous media

An area where partial slip boundary conditions are commonly used as an effective wall model is for simulations over superhydrophobic surfaces. A hydrophobic surface is a “water fearing” surface, i.e., the water tries to minimize the contact with the surface. Furthermore a superhydrophobic surface is a hydrophobic surface having nano-scale roughness on it. This implies water droplets to roll on the surface; see Ma & Hill (2006). A water flow over a superhydrophobic wall boundary implies a layer of air bubbles in the near wall region. Moreover, this bubble layer implies a reduced friction drag on the wall. In numerical simulations, to account for the averaged effect of the bubble layer of an superhydrophobic surface the no-slip boundary condition is usually replaced by a slip boundary condition with parameterized friction coefficients; see Min & Kim (2004).

Moreover, partial slip boundary conditions are also commonly applied in simulations of flows over permeable blocks (or porous media). A permeable material is often approximated by the empirical Darcy’s law that states that the mean velocity $Q$ in the porous media is proportional to the mean stream-wise pressure gradient $dP/dx_3$, i.e., $Q = -(k/\mu)dP/dx_3$, where $k$ is the permeability parameter for the porous material and $\mu$ the viscosity. Thus, Darcy’s law represents the locally averaged velocity through the permeable material rather than the true velocity. In the interface between the permeable block and a turbulent flow above it Beavers & Joseph (1967) suggested to use partial slip boundary conditions to smoothly take into account the boundary layer forming inside the porous media. The boundary conditions they proposed read $du/dx_3 = (\alpha/\sqrt{k})(u - Q)$ where $\alpha$ is an unknown modeling parameter. Saffman (1971) further showed that often in the Beavers–Joseph condition the velocity $Q$ can be negligible to imply a typical slip boundary condition expression.

3.3. Partial slip boundary conditions for LES of atmospheric boundary layers

In atmospheric boundary layer simulations where the Reynolds numbers are very high and the surface is fully rough, the description of the flow at the surface boundary becomes for most real world scenarios extremely complicated. On land the roughness elements are not simple to account for; the turbulence inside trees, grass etc. moves in time and the movements imply a change in the fluid flow around them. For off-shore conditions the water surface may on average be rather flat, but the water moves both in horizontal and vertical directions as traveling waves.
3.3. Partial slip boundary conditions for LES of ABLs

Commonly employed as the simplest alternative in large-eddy simulations of atmospheric boundary layers is the Moeng surface stress model presented in §3.2.2.2. The Moeng model is often a natural choice in ABL LES simulations due to the common usage of finite differences approximations for the wall normal derivatives. However, in codes which does not allow for flux boundary conditions it cannot directly be applied. Furthermore it also has several drawbacks which were also addressed in §3.2.2.2.

We have through this chapter introduced the slip boundary conditions. These are more general than stress models, have much better mathematical support and do allow for a grid independent result. However, they have not found their way into the atmospheric boundary layer community yet. We hereby present some ideas how slip boundary conditions can be used in atmospheric codes and in particular for the Fourier–Chebushev code that is presented in §4.

3.3.1. Log law based slip model

Assume we want to solve the filtered Navier–Stokes equations for a neutral atmospheric boundary layer flow. The flow is expected to be turbulent all the way down to a fully rough surface boundary were we want to impose appropriate wall boundary conditions. Furthermore, the roughness elements are typically smaller than the grid spacing and cannot be meshed. Using slip boundary conditions the averaged effect of roughness can be taken into account through the friction coefficients. This is similar to the ideas of John et al. (2004) and Bose & Moin (2014) who derived effective friction parameters to take into account the filtering effects on smooth boundaries.

We consider a computational box domain $\Omega$ for which we at the lower flat boundary $\Gamma$ want to impose the partial slip boundary conditions for the LES filtered velocities

$$\bar{u}_3 = g, \quad \beta_j \bar{u}_j + \frac{\partial \bar{u}_j}{\partial x_3} = 0, \quad j = 1, 2, \quad \text{on } \Gamma,$$

where $g$ is a possible transpiration velocity. Now, let $\delta h$ define the height of a roughness region $\Omega_r$ including the roughness elements and $h_r$ define the roughness height. A sketch of the particular setup can be seen in Figure 3.2. Like the Moeng model we assume that the rough log law hold for the filtered horizontal velocities. But we fix the height $\delta h$ instead of using a grid dependent height ($z_{1/2}$ in the Moeng model; see §3.2.2.2) such that

$$U(x_3) := \sqrt{\langle \bar{u}_1 \rangle^2 + \langle \bar{u}_2 \rangle^2} = \frac{u_\tau}{\kappa} \log \left( \frac{\delta h + x_3}{h_r} \right), \quad 0 \leq x_3 \leq L_3,$$

with vertical derivative

$$\frac{\partial U}{\partial x_3} = \frac{u_\tau}{\kappa x_3}, \quad 0 \leq x_3 \leq L_3.$$

(3.16)
Wall boundary conditions and wall modeling

Figure 3.2: Configuration for slip boundary conditions of a high Reynolds number flow simulation over a rough wall. Mean streamwise velocity profile are shown in bold line. The region $\Omega$ is the computational domain and the region $\Omega_r$ is a roughness region below the computational (artificial) boundary $\Gamma$. The spanwise axis $x_2$ is pointed into the page.

At $x_3 = 0$ the friction coefficients are now easily computed as

$$\beta_j(\delta h, h_r) = -\frac{\partial U(0)}{\partial x_3} / U(0) = \frac{-1}{\delta h \log (\delta h/h_r)}, \quad j = 1, 2.$$  

(3.19)

It is easy to check that these coefficients satisfy necessary limits of no-slip and free slip. When $\delta h \to h_r$ it follows that $\beta_J \to \infty$ which implies no-slip. And if $\delta h \to \infty$ then $\beta_J \to 0$ which implies free-slip.

Note that the friction coefficients are not dependent on $u_\tau/\kappa$. The boundary conditions make sure that a logarithmic behavior is obtained but do not force the flow to have a specific derivative or a specific velocity at the boundary. No additional empirical parameters are needed other than the heights $\delta h$ and $h_r$.

The roughness height $h_r$ must however be specified. It is usually determined from field measurement data and is the value where a fitted logarithmic curve passes the $x_3$ axis, i.e., where the velocity becomes zero. It is smaller than the height of an individual roughness element and typically around 0.1 meters (for grass) or 0.0001 in non-dimensional units normalized with a boundary layer height of 1000m. According to (3.19) on the other hand, both the size of $\delta h$ and $h_r$ influence the magnitude of a friction coefficient $\beta_j$, which controls the size of a corresponding slip velocity that is obtained given specific vertical derivative. Thus, provided a $\beta_j$, the value of $\delta h$ may be chosen in an ad-hoc way. For a coarse resolution simulation it may be chosen larger than for a fine resolution so that a lower gradient is obtained at the boundary. One may chose $\delta h$ as small as the numerics allow. As a value closer to $h_r$ imply less slip and a higher
3.3. Partial slip boundary conditions for LES of ABLs

...gradient, it becomes more demanding but allows more turbulent scales to be resolved. Tests with different choices of these parameters will be discussed in §5. A paramount difference between these slip boundary conditions and the Moeng model is that we fix $\delta h$ whereas the Moeng model within a staggered grid formulation choses a $\delta h$ dependent on the grid resolution. Thus, with the Moeng model, in order to obtain a reasonably high stress, one must typically change the grid resolution in the first few points whereas with the slip boundary conditions we can change the stress through the parameters $\beta_j$ and $\delta h$ and $h_r$ in a grid independent way.

3.3.2. Boundary conditions for non-neutral conditions

For non neutral conditions it is common practice in the boundary layer meteorology community to employ the Monin–Obukhov similarity theory and derive momentum and heat fluxes for the boundary conditions from so called universal empirical functions; see appendix B. Popular functions are the ones by Businger et al. (1971) fitted from measurement data collected in the open fields of Kansas in 1968, widely called “the Kansas experiment”. These functions are however nonlinear and typically a Newton method must be used to compute the necessary parameters in every time step of a simulation. Thus, the boundary

![Figure 3.3: Businger et al. (1971) approximations of mean horizontal velocity $U/u_r$ (see Equation B.7) plotted for different stability conditions. The dash dotted lines (---) are stably stratified profiles, and the dashed lines (--) are unstably stratified profiles. The stability conditions considered are the Obukhov lengths $L \in \{1, 5, 10\}$ (a higher $|L|$ implies a weaker stratification; see Equation B.3). The roughness height was here chosen as $h_r = 0.1 \text{ m}$ for all cases.](image-url)
conditions become even more computationally unreliable and possibly more expensive.

In Figure 3.3 mean profiles from the Businger universal functions are plotted for different stability conditions. One can note that close to the boundary the functions are all close to neutral for sufficiently high stability. Since the stratification has very little impact on the flow close to the surface where the boundary conditions are imposed, it is indeed questionable to use stability functions instead of just apply the neutral condition for all different stability conditions. In meteorological applications where the grid resolution sometimes is very coarse and the first grid level is located far inside the domain, they may be necessary to be used together with a Moeng like boundary condition. However for the slip boundary conditions where we instead have the possibility to chose $\delta h$ sufficiently small, the neutral boundary conditions would be justified also for stable and unstable conditions. Some numerical results based on this are presented in §5.4.

3.3.3. Boundary conditions on turbulence intensity in Fourier space

Inverse log laws for the horizontal turbulence intensities (mean statistics based on the variances; $u' := u - \langle u \rangle$) are supported by the so called attached eddy hypothesis (Townsend 1956) which states that all eddies that are of size that scales with their distance from the wall would be considered as attached to the wall. Townsend observed that a constant stress region was obtained if the probability density function of the eddies scales as an inverse power law. He obtained the following expressions for the turbulence intensities:

$$\frac{\langle u'_1^2 \rangle}{u^2_r} = B_1 - A_1 \log\left(\frac{x_3}{L_3}\right),$$  \hspace{1cm} (3.20)

$$\frac{\langle u'_2^2 \rangle}{u^2_r} = B_2 - A_2 \log\left(\frac{x_3}{L_3}\right),$$  \hspace{1cm} (3.21)

$$\frac{\langle u'_3^2 \rangle}{u^2_r} = A_3,$$  \hspace{1cm} (3.22)

$$\frac{\langle u'_1 u'_3 \rangle}{u^2_r} = 1.$$  \hspace{1cm} (3.23)

where $u_r$ is the usual friction velocity, $L_3$ is the boundary layer height and $\{A_j\}_{j=1,2,3}$ and $\{B_j\}_{j=1,2}$ are constants. The result is valid close to a wall but just as close that the viscosity can be negligible. Equations (3.20)–(3.23) have been validated to high Reynolds number experiments as well as moderate Reynolds number DNS simulations. Values for the constants fitted to atmospheric boundary layer can be found in Marusic et al. (2013). According to the attached eddy hypothesis this means that only the mean velocity should increase from the wall, not the fluctuations. The magnitudes of the horizontal velocity fluctuations are expected to have the opposite behavior. They decrease from the wall.
Figure 3.4: Attached eddy hypothesis. Eddies that are scaled with their distance from a wall are assumed attached to the wall. Eddies are here approximated as circles.

If the boundary conditions for the filtered instantaneous velocities are based on the mean logarithmic law for both the mean velocity and the fluctuations it is clear that both the mean and the fluctuations will increase in size in the vicinity of the boundary as a consequence of the positive velocity gradients. This means that the mean velocity as well as the turbulence intensity will always be lower at the boundary than some small distance away from it. The maximum turbulence intensity cannot be at the wall and a “spurious peak” will be present as a consequence. This effect is obtained both for slip boundary conditions (results are shown in §5) and for stress boundary conditions as well; see e.g. the results in Mason & Thomson (1992).

In this thesis we employ a Fourier–Chebyshev spectral method (see §4). For such discretization the wall boundary conditions are imposed in Fourier space and there is a possibility to impose boundary conditions on different wavenumbers separately. A planar average $\langle \cdot \rangle$ is then more precisely equal to the Fourier coefficients of the zero streamwise and spanwise wavenumbers. Moreover the fluctuation parts correspond to the bulk of the coefficients of non-zero wavenumbers.

Expanding the filtered velocity vector $\bar{\mathbf{u}}$ in Fourier series over horizontal $x_1 - x_2$ planes yields

$$
\hat{\mathbf{u}}(\mathbf{x}, t) = \sum_{\mathbf{k} \in \mathbb{Z}^2} \hat{\mathbf{u}}(\mathbf{k}, x_3, t) \exp(2\pi i \mathbf{k} \cdot \{x_1/L_1, x_2/L_2\}^\top).
$$

(3.24)
where \( k = (k_1, k_2)^\top \) are the wavenumber indices. We get the following mean velocities and turbulence intensities

\[
\langle \bar{u}_j(x,t) \rangle = \hat{u}_j(0, x_3, t), \quad \langle \bar{u}'_j(x,t)^2 \rangle = \sum_{k \in \mathbb{Z}^2 \setminus 0} \hat{u}^*_j(k, x_3, t) \hat{u}_j(k, x_3, t),
\]

for \( j = 1, 2, 3 \). The asterisk superscript \(*\) denotes here a complex conjugate.

The latter average corresponding to the turbulence intensities follows from the Parseval’s theorem.

We can now deduce friction coefficients for \( \langle \bar{u}'_j^2 \rangle \), \( j = 1, 2 \), based on (3.26) and the attached eddy hypothesis (3.20)–(3.21). For \( \langle \bar{u}_j \rangle \) (or the zero wavenumbers) the friction coefficients given by \( \beta_j = -1/(\delta h \log(\delta h/h_r)) \) which were derived from the rough log law are still used. The partial slip and no penetration boundary conditions (3.16) in Fourier space become:

\[
\begin{align*}
\beta_j \hat{u}_j + \frac{d \hat{u}_j}{dx_3} &= 0, \quad j = 1, 2, \quad k = 0, \text{ on } \Gamma, \quad (3.27a) \\
\gamma_j \hat{u}_j + \frac{d \hat{u}_j}{dx_3} &= 0, \quad j = 1, 2, \quad k \neq 0, \text{ on } \Gamma, \quad (3.27b) \\
\hat{u}_3 &= \hat{g}, \quad \text{on } \Gamma, \quad (3.27c)
\end{align*}
\]

where \( \gamma_j \) denote the friction coefficients for the non-zero wavenumbers. The \( \gamma_j \) are derived as follow. Multiplying (3.27b) with the complex conjugate of \( \hat{u}_j \) we get

\[
\gamma_j \hat{u}^*_j \hat{u}_j + \frac{1}{2} \frac{d}{dx_3} \{ \hat{u}^*_j \hat{u}_j \} = 0, \quad k \neq 0.
\]

After summing up all \( k \neq 0 \) coefficients according to (3.26) it follows that

\[
\gamma_j \langle \bar{u}'_j^2 \rangle + \frac{1}{2} \frac{d}{dx_3} \langle \bar{u}'_j^2 \rangle = 0.
\]

Thus, applying (3.20)–(3.21) the friction coefficients for the non-zero wavenumbers can be chosen as

\[
\gamma_j = -\frac{\frac{d}{dx_3} \langle \bar{u}'_j^2 \rangle}{2 \langle \bar{u}'_j^2 \rangle} = \frac{A_j}{2\delta h(B_j - A_j \log(\delta h/L_3))}, \quad j = 1, 2. \quad (3.28)
\]

3.3.3.1. Modified boundary conditions for the instantaneous velocities

When different friction coefficients are chosen for different wavenumbers the actual boundary condition in physical space will change. However, since we know very little about the complex behavior of the instantaneous flow it is hard to know what to expect from the boundary conditions on the instantaneous velocities.

However, we can easily show what boundary conditions we actually impose. Summing up all coefficients of the boundary conditions we get after some
manipulation:

\[(\beta_j - \gamma_j)\langle \bar{u}_j \rangle + \gamma_j \bar{u}_j + \frac{\partial \bar{u}_j}{\partial x_3} = 0. \quad j = 1, 2, \quad \text{on } \Gamma. \quad (3.29)\]

which can also be written as

\[\beta_j \langle \bar{u}_j \rangle - \gamma_j \bar{u}_j' + \frac{\partial \bar{u}_j}{\partial x_3} = 0. \quad j = 1, 2, \quad \text{on } \Gamma. \quad (3.30)\]

Thus the \(\gamma_j\) have a direct impact on the magnitude of the slip velocity fluctuations \(\bar{u}_j'\).

### 3.3.3.2. Notes about normal velocity boundary conditions

At the boundary \(\Gamma\) the average normal velocity would without problems be taken as zero. As we typically employ a periodic box domain \(\Omega\) with a no stress boundary condition on the upper boundary (see §5.3) this also follows from the continuity equation, which in that case yields:

\[0 = \int_\Omega \nabla \cdot \bar{u} \, d\Omega = \int_{\partial \Omega} \bar{u} \cdot \hat{n} \, dS = \int_\Gamma \bar{u}_3 \, dx_1 dx_2. \quad (3.31)\]

Now, interestingly, according to the attached eddy hypothesis the vertical fluctuations should satisfy \(\langle u_3^2 \rangle = \kappa/\tau\) and \(\langle u_1' u_3' \rangle = 1\). Thus, boundary conditions relaxing the no slip boundary conditions would indeed have a nonzero \(u_3'\). With \(u_3 = 0\) we simply get \(\langle u_1' u_3' \rangle = 0\) which is wrong according to the attached eddy hypothesis. Some preliminary ideas to construct boundary conditions that satisfy these criteria have been discussed but not yet tested out. For now we therefore assumed that there are no vertical motion through the interface and that \(\hat{g}_k = 0\) in (3.27). However, we need to point out, a vertical velocity is important to capture effects of roughness; see also e.g. Orlandi et al. (2006) for more information about this.

### 3.4. Damping/matching functions

The surface boundary conditions presented in §3.3 will not necessarily lead to a perfectly accurate result by themselves. A Robin boundary condition \(\beta_1 \langle \bar{u}_j \rangle + \partial \langle \bar{u}_j \rangle/\partial x_3 = 0\) with \(\beta_1 = -1/(\delta h \log(\delta h/h_\tau))\) does satisfy the rough log law for an unique \(\kappa/\tau\). However, the magnitude of \(\kappa/\tau\) depends on \(\langle \bar{u}_j \rangle\) and \(\partial \langle \bar{u}_j \rangle/\partial x_3\) which on the other hand depend on the near wall stress, that for a LES highly depends on the SGS model.

Unfortunately, most SGS models such as the Smagorinsky model perform rather poorly in regions of high stress, such as in the region close to the wall boundary. For wall bounded flows it is well known that the Smagorinsky model with a constant \(C_S\) value (or a constant Smagorinsky length scale \(l_S = C_S \delta_S\)) becomes severely over-dissipative in the near-wall region (Pope 2001). To solve this issue, external modeling would be introduced. It is common practice in wall bounded LESs to apply a so called damping function to correct the Smagorinsky length scale \(l_S\) to yield a improved near wall performance.
A damping function \( f(x_3) \) can be defined a local scaling of the Smagorinsky length scale with the purpose of smoothly merge together some near wall definition of \( l_S \) with the original Smagorinsky length scale, i.e., \( l_S(x) \to f(x_3)l_S(x) \).

### 3.4.1. van Driest wall damping

The most well known damping function is probably the one proposed in Van Driest (1956), which has been widely used in wall resolved LES; see e.g. Moin & Kim (1982).

In the viscous sublayer the mean velocity components scales as \( \langle u_1 \rangle, \langle u_2 \rangle \propto x_3 \) and \( \langle u_3 \rangle \propto x_3^2 \) and the stresses as \( \langle \tau_{13} \rangle, \langle \tau_{23} \rangle \propto x_3^3 \). This is simply shown by Taylor expanding the quantities and applying the no-slip boundary conditions together with the continuity equation. From these estimates it now directly follows that \( \langle \tau_{ji} \rangle = \langle \nu_t \rangle \partial_3 \langle u_j \rangle \propto \langle \nu_t \rangle \propto x_3^{3/2} \) for \( j = 1, 2 \). We then have \( \langle \nu_t \rangle = l_S^2 \sqrt{\partial_3 \langle u_1 \rangle^2 + \partial_3 \langle u_1 \rangle^2} \), which yields \( l_S \propto x_3^{3/2} \). The problem here is that if the Smagorinsky model is used, then the length-scale \( l_S = C_S \delta_S \neq 0 \) is a constant (assuming \( C_S \) and \( \delta_S \) are constants). This does not agree with the estimate \( l_S \propto x_3^{3/2} \) in the viscous sublayer.

To reduce \( l_S \), van Driest proposed the following damping function

\[
 f_{vD}(x_3) = 1 - \exp \left( \frac{-x_3^3}{26} \right). \tag{3.32}
\]

which tend to one for large viscous units \( x_3^+ := x_3 u_{\tau}/\nu \) and zero as \( x_3 \to 0 \).

### 3.4.2. Mason et al. matching function

In atmospheric boundary layer simulations where the inner region is not resolved, a length scale function proposed in Mason & Callen (1986) and Mason & Thomson (1992) is often used. With the van Driest damping function the aim was to match the viscous sublayer scaling with the inertial range based scaling of the Smagorinsky model. In the Mason et al. model it is instead the logarithmic region scaling, i.e., the mixing length \( l_{ml}(x_3) := \kappa x_3 \), that is matched. For \( \delta h \gg h_r \) and \( x_3 \in [0, L_3] \) the matching proposed by Mason et al. yields

\[
 \frac{1}{l_S(x_3)^\alpha} = \frac{1}{l_0^\alpha} + \frac{1}{l_{ml}(x_3 + \delta h)^\alpha}, \quad \alpha \in \mathbb{R}^+. \tag{3.33}
\]

where the constant \( \alpha \) determines the steepness of the matching. Furthermore, \( l_0 \) defines a fixed Smagorinsky length scale given by

\[
 l_0 := C_S \delta_{\text{max}}, \quad \text{where} \quad \delta_{\text{max}} := \left[ \delta_1 \delta_2 \max_{x_3} \left( \delta_3(x_3) \right) \right]^{1/3}.
\]

Equation (3.33) may, more conveniently, be rewritten as

\[
 l_S(x_3) = \left[ l_0^\alpha + l_{ml}(x_3 + \delta h)^{-\alpha} \right]^{-1/\alpha}, \quad \alpha \in \mathbb{R}^+. \tag{3.34}
\]

Length scale functions \( l_S \) for a typical mesh of \( 64^2 \times 65 \) plotted for different \( \alpha \) in Figure 3.5.

\footnote{Here we introduced the short hand notation \( \partial_3 := \partial/\partial x_3 \).}
3.4. Damping/matching functions

A downside of the Mason matching is that for small $\alpha$ the asymptotics $l_0$ and $l_{\text{mix}}$ cannot be accurately obtained. This is seen Figure 3.5b. With $\alpha = 1$ one clearly see some deviation, and with $\alpha = 0.5$ the result is not sufficient for practical use.

Figure 3.5: Smagorinsky length scales modified using the Mason et al. matching function plotted for $\kappa = 0.4$, $\delta h/L_3 = 0.0029$ ($\beta \approx 50$), $C_s = 0.1$, $\delta_{\text{max}} = 0.098$ (corresponding to a $64^2 \times 65$ point grid with Chebyshev–Gauss–Lobatto grid point distribution in $x_3$) and different matching parameters $\alpha$. 
Chapter 4

Numerical method

In this chapter we describe the spectral discretization methods that we use to solve the LES equations. The incompressible Navier–Stokes equations in the normal-velocity normal-vorticity formulation is presented in section 4.1. The temporal and spatial discretization methods are presented in sections 4.2. A detailed description of how we impose boundary conditions in the vertical inhomogeneous direction is further discussed in section 4.3. The end of the chapter is devoted to two short sections about high Reynolds number treatment and the discretization of the scalar equation.

The method presented in this chapter is based on a code developed at KTH Mechanics. The new work in this thesis regards the new boundary condition implementation presented in §4.3. More information about the original code can be found in Lundbladh et al. (1999) and Chevalier et al. (2007).

4.1. The normal-velocity normal-vorticity formulation

Considering 3D incompressible flows over horizontally homogeneous directions, the Navier–Stokes equations can be solved efficiently using direct solution methods in the Fourier domain assuming periodic boundary conditions are appropriate. A common mathematical formulation in this context is the normal-velocity normal-vorticity formulation, first utilized in Orszag & Patera (1980) and moreover used in the famous Kim et al. (1987), Reτ = 180, channel flow paper.

4.1.1. Horizontally homogeneous form

Assuming a box domain Ω_{box} = Ω_{⊥} × [0, L_3] where the flow is periodic over the horizontal planes Ω_{⊥} := [0, L_1] × [0, L_2] and inhomogeneous in the vertical direction x_3 ∈ [−1, 1], the incompressible Navier–Stokes equations can be
4.1. The normal-velocity normal-vorticity formulation

written as a horizontally homogeneous initial boundary value problem

\[
\begin{aligned}
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{N}(\mathbf{u}) + \nabla q - \nu \Delta \mathbf{u} &= 0, & \text{in } \Omega \times (0, T), \\
\nabla \cdot \mathbf{u} &= 0, & \text{in } \Omega \times (0, T), \\
\mathbf{u} &= \mathbf{u}_0(x), & \text{in } \Omega \times \{t = 0\}, \\
\mathbf{u}(x + L_j \mathbf{e}_j, t) &= \mathbf{u}(x, t), \; j = 1, 2, & \text{on } \mathbb{R} \times (-1, 1) \times (0, T), \\
q(x + L_j \mathbf{e}_j, t) &= q(x, t), \; j = 1, 2, & \text{on } \mathbb{R} \times (-1, 1) \times (0, T), \\
\mathcal{B} \mathbf{u} &= 0, & \text{on } \Omega_\perp \times \{0, L_3\},
\end{aligned}
\]

where

\[\mathbf{N}(\mathbf{u}) := \omega \times \mathbf{u} - \mathbf{f},\]

defines the nonlinear term together with an external forcing function \(\mathbf{f}\). This term will be treated with an explicit time discretization (see §4.2.2). Moreover, in (4.1a) \(q := p + \frac{1}{2} \|\mathbf{u}\|^2 \) is a modified pressure obtained using the rotational form of the nonlinear term, and \(\mathcal{B}\) a boundary operator for the vertical boundary planes that would be of Dirichlet, Neumann or Robin type. The rotation form provides better conservation properties and is also cheaper to compute and more numerically stable for lower viscosities than the usual convective form \(\mathbf{u} \cdot \nabla \mathbf{u}\) (see also Canuto et al. 1988).

The divergence of the subgrid-scale tensor for large eddy simulation \(\nabla \cdot \mathbf{T}_u\) is included in the forcing function \(\mathbf{f}\) and therefore inside \(\mathbf{N}(\mathbf{u})\). More about the LES part is explained in §4.4. We do not explicitly write out any overbar quantities for LES in this chapter. The discretization will be performed similarly for the filtered or unfiltered equations except for the treatment of \(\mathbf{N}(\mathbf{u})\) which is performed with an explicit time-discretization and thus treated separately.

4.1.2. Normal-velocity–normal-vorticity equations

Applying the curl operator \((\nabla \times)\) to (4.1a) yields the vorticity equation

\[
\frac{\partial \omega}{\partial t} - \nu \Delta \omega + \nabla \times \mathbf{N}(\mathbf{u}) = 0.
\]

The vorticity equation (4.3) does not depend on pressure since \(\nabla \times \nabla q = 0\) and could in principle be solved instead of the incompressible Navier–Stokes equations in the usual \((\mathbf{u}, p)\) form. No continuity equation for vorticity needs to be included since \(\nabla \times \nabla \cdot \mathbf{v} = 0\) for any vector \(\mathbf{v} \in \mathbb{R}^3\). An initial condition for the vorticity can be computed from the initial velocity field. The vorticity equation has however six dependent variables instead of four, but treating \(\mathbf{N}(\mathbf{u})\) explicitly in the time discretization this problem can also be eliminated in practice. The remaining problem is that boundary conditions on vorticity typically are cumbersome.
In the normal-velocity normal-vorticity formulation the vertical component of the vorticity equation is used. That is,
\[ \partial_t \omega_3 - \nu \Delta \omega_3 + \nabla \times \left[ N(u) \cdot e_3 \right] = 0 \quad (4.4) \]
where \( e_3 = (0, 0, 1) \). Note that the normal vorticity is a function on the horizontal velocities \( u_1 \) and \( u_2 \). Thus the normal vorticity equation is representative for the horizontal velocity quantities.

Furthermore, an equation for the vertical velocity can be derived together with the elimination of the pressure term by applying the Laplacian operator to (4.1a). First, as is commonly employed in the numerical treatment of the Navier–Stokes equations, applying the divergence operator to (4.1a) and using the continuity equation (4.1b) yields a Poisson equation for pressure:
\[ \Delta q = -\nabla \cdot N(u). \quad (4.5) \]
Moreover, applying the Laplacian to (4.1a) and keeping the \( x_3 \) equation only yields a fourth order equation for the normal velocity:
\[ \frac{\partial}{\partial t} \Delta u_3 - \nu \Delta^2 u_3 + \Delta \left[ N(u) \cdot e_3 \right] - \frac{\partial}{\partial x_3} \left[ \nabla \cdot N(u) \right] = 0 \quad (4.7) \]
where \( \Delta^2 := \Delta(\Delta) \). Equations (4.4) and (4.7) are the governing equations in normal-velocity normal-vorticity formulation, valid for the fluctuating quantities (not for the horizontal mean; see §4.1.3).

### 4.1.3. Equations in Fourier/Fourier/physical space

Expanding \( u_3 \) and \( \omega_3 \) in Fourier series over the periodic planes \( x_1 - x_2 \) we get
\[ u_3(x, t) = \sum_{k \in \mathbb{Z}^2} \hat{u}_3(k, x_3, t) e^{i(K \cdot x)}, \quad (4.8) \]
\[ \omega_3(x, t) = \sum_{k \in \mathbb{Z}^2} \hat{\omega}_3(k, x_3, t) e^{i(K \cdot x)}, \quad (4.9) \]
where \( k = (k_1, k_2)^\top \) and \( K = (K_1, K_2, K_3)^\top := (2\pi k_1/L_1, 2\pi k_2/L_2, 0)^\top \) are dual variables (wavenumbers).

The horizontal velocity components \( u_1 \) and \( u_2 \) are found from the continuity equation and the definition of normal vorticity
\[ \frac{\partial u_3}{\partial x_3} = -\frac{\partial u_1}{\partial x_1} - \frac{\partial u_2}{\partial x_2}, \quad \text{and} \quad \omega_3 = \frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2}. \]
Expressing these in terms of the Fourier coefficients gives
\[ \frac{d\hat{u}_3}{dx_3} = -iK \cdot \hat{u}, \quad \text{and} \quad \hat{\omega}_3 = iK \cdot \hat{u}, \]
4.1. The normal-velocity normal-vorticity formulation

which after some manipulation yields expressions for the Fourier coefficients of the horizontal velocities

\[
\hat{u}_1 = \frac{i}{|K|^2} \left( K_1 \frac{d\hat{u}_3}{dx_3} - K_2 \hat{\omega}_3 \right), \tag{4.10}
\]

\[
\hat{u}_2 = \frac{i}{|K|^2} \left( K_1 \hat{\omega}_3 + K_2 \frac{d\hat{u}_3}{dx_3} \right). \tag{4.11}
\]

**Remark 4.1.** In (4.10)–(4.11) there is a singularity for \( |K| = 0 \). Hence, \( \hat{u}_1 \) and \( \hat{u}_2 \) cannot be obtained for \( k = 0 \). An alternative is to solve for the zero wavenumber solutions from separate equations (see §4.1.4).

However, in the \( k \neq 0 \) case a substitution of (4.8)–(4.9) into the normal-velocity and normal-vorticity equations (4.4) and (4.7) yield due to the orthogonality of the Fourier basis the following equations for the Fourier coefficients

\[
\begin{cases}
\frac{\partial \hat{\omega}_3}{\partial t} - \nu D_k^2 \hat{\omega}_3 + i K^\perp \cdot \hat{N}_k(u) = 0, \tag{4.12a} \\
\frac{\partial \hat{u}_3}{\partial t} - \nu D_k^4 \hat{u}_3 + D_k^2 \left[ \hat{N}_k(u) \cdot e_3 \right] - \frac{\partial}{\partial x_3} \left[ D_k \cdot \hat{N}_k(u) \right] = 0, \tag{4.12b}
\end{cases}
\]

where \( K^\perp := (K_2, -K_1, 0)^\top \) are the horizontal wavenumbers, \( D_k := (iK_1, iK_2, \partial/\partial x_3)^\top \) a horizontal gradient operator, \( D_k^2 := D_k^\top D_k = -|K|^2 + \partial^2/\partial x_3^2 \) the representation for the Laplacian, \( D_k^4 := (D_k^2)^\top D_k^2 \) is the fourth order operator and the subscript \( k \) emphasizes wavenumber dependency.

4.1.4. Equations for planar averages

Since \( \hat{u}_1 \) and \( \hat{u}_2 \) cannot be obtained from (4.12a)-(4.12b) for \( K = 0 \) the equations, (4.12a)–(4.12b) are supplemented with specific equations for these the zero wavenumber quantities.

First of all, since the horizontal derivatives of the planar averages are zero, it directly follows from the continuity equation that for all \( x_3 \in [0, L_3] \) and \( t \geq 0 \) we have

\[
\frac{\partial \hat{u}_3}{\partial x_3} (k = 0, x_3, t) = 0, \tag{4.13}
\]

Thus the mean vertical quantity can be set equal to a Dirichlet boundary condition

\[
\hat{u}_3(k = 0, 0, t) = \hat{u}_3(k = 0, L_3, t) = \text{constant}. \tag{4.14}
\]

Furthermore, taking planar averages of the full momentum equation (4.1a) for the horizontal quantities we obtain for \( k = 0 \) that

\[
\frac{\partial \hat{u}_j}{\partial t} - \nu \frac{\partial^2 \hat{u}_j}{\partial x_3^2} + \hat{N}_0(u) \cdot e_j = 0, \quad j = 1, 2. \tag{4.15}
\]
4. Numerical method

4.1.5. Summary – The continuous problem

The full continuous problem for the normal velocity normal vorticity in Fourier-Fourier-physical space can now be stated as follows. For \( k \neq 0 \) we have:

\[
\begin{align*}
\frac{\partial \hat{\omega}_3}{\partial t} - \nu D_k^2 \hat{\omega}_3 + iK_{\perp} \cdot \hat{N}_k(u) &= 0, \\
\frac{\partial \hat{u}_3}{\partial t} - \nu D_k^4 \hat{u}_3 + D_k^2 [\hat{N}_k(u) \cdot e_3] - \frac{\partial}{\partial x_3} [D_k \cdot \hat{N}_k(u)] &= 0, \\
D_k \cdot \hat{u} &= 0, \quad (4.16a) \\
\hat{u}_3(k, x_3, 0) &= \hat{u}_{3,0}, \quad \hat{\omega}_3(k, x_3, 0) = \hat{\omega}_{3,0}, \\
B_k^{u_3} \hat{u}_3 &= 0, \quad B_k^{\omega_3} \hat{\omega}_3 = 0, \\
\end{align*}
\]

And for \( k = 0 \):

\[
\begin{align*}
\frac{\partial \hat{u}_j}{\partial t} - \nu \frac{\partial^2 \hat{u}_j}{\partial x_3^2} + \hat{N}_0(u) \cdot e_j &= 0, \quad j = 1, 2, \\
\hat{u}(0, x_3, 0) &= \hat{u}_0, \quad (4.17a) \\
B_0^{u_j} \hat{u}_j &= 0, \quad j = 1, 2, \\
\hat{u}_3 &= \text{constant}, \quad (4.17d)
\end{align*}
\]

In (4.16e) and (4.17c) \( B_k^{u_3}, B_k^{\omega_3} \) and \( B_0^{u_j}, j = 1, 2 \) are appropriate boundary operators.

4.2. Temporal and spatial discretizations

We now we review the discretization methods we use to solve the normal-velocity normal-vorticity problem.

4.2.1. Horizontal spatial discretization – Fourier approximations

For the horizontal space discretization the spectral approximation is to find a truncated approximation to the infinite sums (4.8) and (4.9)

\[
\begin{align*}
u_{3,N}(x, t) &= \sum_{k \in S_N} \hat{u}_3(k, x_3, t)e^{i(K \cdot x)}, \\
\omega_{3,N}(x, t) &= \sum_{k \in S_N} \hat{\omega}_3(k, x_3, t)e^{i(K \cdot x)} \\
\end{align*}
\]

where

\[
S_N := \{k \in \mathbb{Z}^2: \|k_j\| \leq N_j/2 - 1, \ j = 1, 2\}.
\]
A Fourier spectral approximation to (4.16)–(4.17) can now be written as follows. For \( k \in S_N \setminus 0 \) we have:

\[
\begin{aligned}
\frac{\partial \hat{\omega}_3}{\partial t} - \nu D^2_{kN} \hat{\omega}_3 + iK^\perp \cdot \hat{N}_k(u_N) &= 0, \\
\frac{\partial \hat{u}_3}{\partial t} - \nu D^4_{kN} \hat{u}_3 + D^2_k [\hat{N}_k(u_N) \cdot e_3] - \frac{\partial}{\partial x_3} [D_k \cdot \hat{N}_k(u)] &= 0,
\end{aligned}
\]

(4.20a)

\[
\begin{aligned}
\hat{D}_k \cdot \hat{u} &= 0, \\
\hat{u}_3(k, x_3, 0) &= \hat{u}_{3,0}, \\
\hat{\omega}_3(k, x_3, 0) &= \hat{\omega}_{3,0},
\end{aligned}
\]

(4.20b)

And for \( k = 0 \):

\[
\begin{aligned}
\frac{\partial \hat{u}_j}{\partial t} - \nu \frac{\partial^2 \hat{u}_j}{\partial x_3^2} + \hat{N}_0(u_N) \cdot e_j &= 0, \quad j = 1, 2, \\
\hat{u}(0, x_3, 0) &= \hat{u}_0, \\
\hat{B}_k^{u_3} \hat{u}_3 &= 0, \\
\hat{u}_3 &= \text{constant},
\end{aligned}
\]

(4.21a)

(4.21b)

(4.21c)

The main differences here aside from the truncated wavenumber ranges, is that the nonlinear terms are based on approximate velocities \( u_N = (u_{1N}, u_{2N}, u_{3N})^T \) where the horizontal quantities may be written similarly as (4.18) and (4.19). In practice, since these terms are treated explicitly in time, they are calculated using the transformations (4.10)–(4.11).

### 4.2.2. Temporal discretization

At a discrete time \( t = t^n \) we define \( \phi_N^O(x) := \phi_N(x, t^n) \) and \( \hat{\phi}^n(k, x_3) := \hat{\phi}(k, x_3, t^n) \), where \( \phi \) can be any quantity. Furthermore we define the time step-size as \( \delta t \) such that \( t^{n+1} = t^n + \delta t \).

The time integration is treated with a low storage Runge–Kutta/Crank-Nicholson scheme. Linear diffusion terms are discretized implicitly with a second order Crank–Nicolson method and the nonlinear and forcing terms are treated with an explicit Runge–Kutta substepping of either 3rd or 4th order. Applying the Crank–Nicolson scheme to the momentum equations of (4.20)–(4.21) we get for \( k \in S_N \setminus 0 \)

\[
\begin{aligned}
\left( 1 - \frac{\nu \delta t}{2} D_k^2 \right) \hat{\omega}_3^{n+1} &= \left( 1 + \frac{\nu \delta t}{2} D_k^2 \right) \hat{\omega}_3^n - \delta t f_k(u_N^n), \\
\left( 1 - \frac{\nu \delta t}{2} D_k^2 \right) D_k^2 \hat{u}_3^{n+1} &= \left( 1 + \frac{\nu \delta t}{2} D_k^2 \right) D_k^2 \hat{u}_3^n - \delta t g_k(u_N^n),
\end{aligned}
\]

(4.22a)

(4.22b)

and for \( k = 0 \)

\[
\begin{aligned}
\left( 1 - \frac{\nu \delta t}{2} D_k^2 \right) \hat{u}_j^{n+1} &= \left( 1 + \frac{\nu \delta t}{2} D_k^2 \right) \hat{u}_j^n - \delta t h_{0,j}(u_N^n), \quad j = 1, 2.
\end{aligned}
\]

(4.23)
In (4.22)–(4.23) we introduced the following functions for the explicit time-

discretization:

\[
\begin{align*}
  f_k(u^n_N) & := iK^\perp \cdot N_k(u^n_N), \\
  g_k(u^n_N) & := D_k^2 [N_k(u^n_N) \cdot e_3] - \frac{\partial}{\partial x_3} [D_k \cdot N_k(u^n_N)], \\
  h_{0,j}(u^n_N) & := N_0(u^n_N) \cdot e_j, \quad j = 1, 2.
\end{align*}
\]

Now we apply the Runge–Kutta method to (4.22)–(4.23). It is then necessary to

introduce a second index \(m\) for intermediate sub-steps (three for RK3 and four

for RK4) such that \(t_{n,m} = t_n + c_m \delta t \in [t^n, t^{n+1})\). Then \(\alpha_m := c_m - c_{m-1}\)

becomes the fraction of the full time step \(\delta t\) for each sub-step \((t_{n,m} - t_{n,m-1} = \alpha_m \delta t)\). For

simplicity we furthermore let \(\phi^{n,m} := \phi(k, x_3, t^n_m)\). Runge–Kutta weights are

given by \(\{b_l\}_{l=0}^{m-1}\) and have pre-defined sizes between zero and one; see Chevalier

et al. (2007). The full time-discretization for (4.22)-(4.23) can now be stated. For \(k \in S_N \setminus 0\) we have

\[
\begin{align*}
  \left( 1 - \frac{\nu \alpha_m \delta t}{2} D_k^2 \right) \hat{\omega}^{n,m}_3 &= \left( 1 + \frac{\nu \alpha_m \delta t}{2} D_k^2 \right) \hat{\omega}^{n,m-1}_3 \\
  &- \alpha_m \delta t \sum_{l=0}^{m-1} b_{m,l} f_k(u^{n,m-1}_N), \quad (4.27a) \\
  \left( 1 - \frac{\nu \alpha_m \delta t}{2} D_k^2 \right) D_k^2 \hat{u}^{n,m}_3 &= \left( 1 + \frac{\nu \alpha_m \delta t}{2} D_k^2 \right) D_k^2 \hat{u}^{n,m-1}_3 \\
  &- \alpha_m \delta t \sum_{l=0}^{m-1} b_{m,l} g_k(u^{n,m-1}_N). \quad (4.27b)
\end{align*}
\]

And for \(k = 0\):

\[
\begin{align*}
  \left( 1 - \frac{\nu \alpha_m \delta t}{2} D_k^2 \right) \hat{u}^{n,m}_j &= \left( 1 + \frac{\nu \alpha_m \delta t}{2} D_k^2 \right) \hat{u}^{n,m-1}_j \\
  &- \alpha_m \delta t \sum_{l=0}^{m-1} b_{m,l} h_{0,j}(u^{n,m-1}_N), \quad j = 1, 2. \quad (4.28)
\end{align*}
\]

4.2.3. Normal spatial direction – Chebyshev spectral approximations

Recall that in (4.27a)–(4.28) we have the Laplacian operators \(D_k^2 = -|K|^2 + \partial^2/\partial x_3^2\) where \(\partial^2/\partial x_3^2\) is still in continuous form. The discretization in the

inhomogeneous \(x_3\) direction is performed with a Chebyshev-series expansion. However, before proceeding by applying the Chebyshev-spectral approximation

we simplify the equations, moving all parts that are treated with an explicit
time-discretization to the right hand side of the equations (4.27)–(4.28). For
4.2. Temporal and spatial discretizations

\[ k \in S_N \setminus \{0\} \text{ we get:} \]

\[
\begin{align*}
\left\{ \begin{array}{l}
\left( \frac{d^2}{dz_3^2} - \lambda_k^m \right) \hat{\omega}_n^m = F_{k}^{n,m-1}, \\
\left( \frac{d^2}{dz_3^2} - \lambda_k^m \right) D_k^{n,m} = G_{k}^{n,m-1},
\end{array} \right.
\end{align*}
\]

and for \( k = 0 \):

\[
\left( \frac{d^2}{dz_3^2} - \lambda_k^m \right) \hat{u}_j^m = H_{0,j}^{n,m-1}, \quad j = 1, 2.
\]

where \( \lambda_k^m := 2/(\nu \alpha_m \delta t) - |K|^2 \). The explicit right hand sides here are

\[
\begin{align*}
F_{k}^{n,m-1} &:= -\frac{2}{\nu \alpha_m \delta t} \alpha_m \delta t \sum_{l=0}^{m-1} b_{m,l} f_k(u_{N}^{n,m-1}), \\
G_{k}^{n,m-1} &:= -\frac{2}{\nu \alpha_m \delta t} \alpha_m \delta t \sum_{l=0}^{m-1} b_{m,l} g_k(u_{N}^{n,m-1}), \\
H_{0,j}^{n,m-1} &:= -\frac{2}{\nu \alpha_m \delta t} \alpha_m \delta t \sum_{l=0}^{m-1} b_{m,l} h_{0,j}(u_{N}^{n,m-1}).
\end{align*}
\]

The equations (4.29a) and (4.30) are second order ordinary differential equations of similar structure and can easily be solved analytically or numerically with a spectral approximation provided boundary conditions are given. An efficient way is to use the Chebyshev-tau method, which is presented below. However the fourth order equation (4.29b) for the normal velocity is not as straightforward to solve. As is pointed out by Gottlieb and Orszag (1977) it leads to ill-conditioned system matrices. Also, the condition number of a fourth order Chebyshev differential operator becomes high; see e.g. Shen (1994). However, instead of solving (4.29b) directly Kim et al. (1987) split it up into two second order systems that are solved in a two step procedure without dealing with the severe accuracy loss. The splitting is done by introducing an auxiliary variable \( \Phi = D_k^{n,m} \) which rewrites (4.29b) as follows:

\[
\begin{align*}
\left\{ \begin{array}{l}
\left( \frac{d^2}{dz_3^2} - \lambda_k^m \right) \Phi = G_{k}^{n,m-1}, \quad k \in S_N \setminus \{0\}, \quad \quad (4.34a) \\
\left( \frac{d^2}{dz_3^2} - |K|^2 \right) \hat{u}_3^m = \Phi, \quad k \in S_N \setminus \{0\},
\end{array} \right.
\end{align*}
\]

which can be solved provided boundary conditions for both \( \Phi \) and \( \hat{u}_3 \) are given.

4.2.3.1. Superposition of solutions

We now deal with several linear second order problems to solve. A solution to a second order linear ODE can be written as a superposition of particular and homogeneous solutions. If supplied with boundary conditions the equations
(4.29a), (4.30), (4.34a), and (4.34b) all become boundary value problems on the following form

\[
\begin{cases}
\frac{d^2 \varphi}{dx_3^2} - \lambda \varphi = f, & -1 < x_3 < 1, \\
B^- \varphi(-1) = B^+ \varphi(1) = 0,
\end{cases}
\] (4.35a)

where \(\lambda\) is a positive constant and \(B^\pm\) are linear boundary operators that may be of either Dirichlet or Neumann type\(^1\).

Now, recall the principle of superposition: If \(\varphi^p\) is an arbitrary (particular) solution to (4.35a) and \(\varphi^h_1(x_3)\) and \(\varphi^h_2(x_3)\) are solutions to the homogeneous form of (4.35a), i.e., (4.35a) with \(f = 0\), then the general solution can be written as

\[
\varphi(x_3) = \varphi^p(x_3) + c_1 \varphi^h_1(x_3) + c_2 \varphi^h_2(x_3),
\]

where \(\{c_j\}_{j=1}^2\) are unknown coefficients.

The superposition of solutions makes it possible to solve a second order linear ODE analytically from arbitrary homogeneous and particular solutions. An unique solution is obtained by applying appropriate boundary conditions to solve for the unknown coefficients. Thus in order to apply appropriate boundary conditions for our systems we need to solve several boundary value problems like (4.35) to obtain as many homogeneous and particular solutions we need to impose sufficiently many boundary conditions.

4.2.3.2. The Chebyshev-tau approximation to (4.35)

An accurate and efficient way to solve the second order problems with constant coefficients is to use the Chebyshev-tau method (Lanczos 1938). A Chebyshev spectral approximation to (4.35) is a truncated Chebyshev series expansion to the continuous solution \(\varphi(x)\)

\[
\varphi_N(x_3) := \sum_{j=0}^{N} \tilde{\varphi}_j T_j(x_3),
\] (4.36)

where \(\{\tilde{\varphi}_j\}_{j=0}^N\) is the set of unknown expansion coefficients and

\[
T_j(x_3) = \cos(j \arccos(x_3)), \quad j = 0, 1, \ldots, N, \quad x_3 \in [-1, 1],
\] (4.37)

the corresponding Chebyshev basis functions. A Chebyshev-tau approximation is similar to the more general Galerkin approximation except in the way it treats boundary conditions. For the Chebyshev-tau method, boundary conditions do not necessary satisfy the basis functions themselves (for the traditional Galerkin approximation to (4.35) expanded in Chebyshev polynomials should requires \(B^\pm T_j(x_3)(\pm 1) = 0\) for each \(j\)). Instead appropriate boundary conditions are enforced by replacing rows in the obtained system matrix of the discretization.

\(^1\)Equation (4.35) with Dirichlet and Neumann boundary conditions is well posed provided that the coefficient \(\lambda\) is positive. Mixed boundary conditions are also well posed but are more tricky to use together with the Chebyshev-tau method; see Canuto et al. (2012).
4.2. Temporal and spatial discretizations

The Galerkin approximation to (4.35) is derived from the variational form where test and trial functions are chosen in the same function space; here as Chebyshev polynomials. For the Chebyshev basis functions \( \{ T_j(x) \}_{j=0}^N \) we get:

\[
\langle \frac{d^2 \varphi_N}{dx^2} - \lambda \varphi_N - f , T_k \rangle_w = 0, \quad k = 0, 1, \ldots, N. \tag{4.38}
\]

where \( \langle p, q \rangle_w = \int_{-1}^{1} p(\eta) q(\eta) \, w(\eta) \, d\eta \) is a weighted \( L_2 \) inner product that for Chebyshev polynomials has \( w(\eta) = \frac{1}{\sqrt{1-\eta^2}} \) to yield the orthogonality \( \langle T_k, T_l \rangle = c_k \delta_{kl} \) where \( c_k \) is a constant value. Expanding each of the individual terms in (4.35) in Chebyshev polynomials and substituting them in (4.38) further leads to:

\[
\sum_{j=0}^{N} \left( \tilde{\varphi}_j^{(2)} - \lambda \tilde{\varphi}_j - \tilde{f}_j \right) \langle T_j, T_k \rangle_w = 0, \quad k = 0, 1, \ldots, N \tag{4.39}
\]

where \( \{ \tilde{\varphi}_j^{(2)} \}_{j=0}^N \) are the coefficients for the expansion of \( \frac{d^2 \varphi_N}{dx^2} \). Due to the orthogonality of the Chebyshev polynomials (4.39) reduces to

\[
\tilde{\varphi}_k^{(2)} - \lambda \tilde{\varphi}_k = f_k, \quad k = 0, 1, \ldots, N. \tag{4.40}
\]

Now, for a Chebyshev-tau method two equations in the Galerkin approximation (4.40) are replaced by boundary conditions:

\[
\begin{cases}
\sum_{j=0}^{N} \tilde{\varphi}_j B^- T_j(-1) = 0, \\
\sum_{j=0}^{N} \tilde{\varphi}_j B^+ T_j(1) = 0
\end{cases} \tag{4.41a}
\]

The coefficients of the second derivative \( \{ \tilde{\varphi}_j^{(2)} \}_{j=0}^N \) can be found from the recurrence relation \( c_k \tilde{\varphi}_j^{(q)} = \tilde{\varphi}_j^{(q)} + 2(k + 1) \tilde{\varphi}_j^{(q-1)} \), where \( q \) is the order of the derivative and \( c_k \) a constant. This is a direct consequence of the Chebyshev polynomials (see Canuto et al. 1988, p. 68). Using the recursive relation in (4.41a), one obtains a quasi tridiagonal system, where the first two rows are replaced with the boundary conditions which can be solved from bottom and up by Gaussian elimination

\[
\begin{align*}
\sum_{j=0}^{N} \tilde{\varphi}_j B^- T_j(-1) &= 0, \\
\sum_{j=0}^{N} \tilde{\varphi}_j B^+ T_j(1) &= 0, \\
\sum_{j \in \{ k-2, k, k+2 \}} \alpha_j \tilde{\varphi}_j &= \sum_{j \in \{ k-2, k, k+2 \}} \beta_j \tilde{f}_j, \quad k = 2, \ldots, N,
\end{align*} \tag{4.42}
\]
4. Numerical method

where

\[ \alpha_{k-2} := \frac{c_{k-2}\lambda}{4k(k-1)}, \quad \alpha_k := \left( 1 - \frac{\lambda \gamma_k}{2(k^2 - 1)} \right), \quad \alpha_{k+2} := \frac{\lambda \gamma_{k+2}}{4k(K+1)} \]

\[ \beta_{k-2} := -\frac{c_{k-2}}{4k(k-1)}, \quad \beta_k := \frac{\gamma_k}{2(k^2 - 1)}, \quad \beta_{k+2} := \frac{\gamma_{k+2}}{4k(k+1)} \]

with

\[ \gamma_k := \begin{cases} 1, & 0 \leq k \leq N - 2, \\ 0, & k > N - 2. \end{cases} \]

Note that the even and odd parts of the (4.42) are uncoupled. Thus it is possible to divide up into two separate sub-systems, one for the odd coefficients and one for the even. An example of the structure can be seen in an example here below. The cost of the direct method for both the odd and even parts is $16N$ assuming that the coefficients $\alpha_k$ and $\beta_k$ are pre-computed. For more details see Canuto et al. (1988).

Example 4.1. Suppose now we want to solve (4.35) with the inhomogeneous Dirichlet boundary conditions $\varphi(-1) = a$ and $\varphi(1) = b$. For Dirichlet boundary conditions the boundary operators becomes $B^- = B^+ = 1$ and the Chebyshev polynomials at the boundaries simply become $T_j(-1) = (-1)^j$, and $T_j(1) = 1$ for $j = 0, 1, \ldots, N$. The linear systems for the even and odd parts for this case then takes the following forms

\[
\begin{bmatrix}
1 & 1 & 1 & \ldots & 1 \\
\alpha_0 & \alpha_2 & \alpha_4 & \alpha_6 & \\
\alpha_2 & \alpha_4 & \alpha_6 & \ddots & \\
\alpha_{N-4} & \alpha_{N-2} & \alpha_{N-2} & \ddots & \\
\alpha_{N-2} & \alpha_N & & & \\
\end{bmatrix}
\begin{bmatrix}
\tilde{\varphi}_0 \\
\tilde{\varphi}_2 \\
\tilde{\varphi}_4 \\
\vdots \\
\tilde{\varphi}_N \\
\end{bmatrix}
= 
\begin{bmatrix}
\frac{1}{2}(a + b) \\
\beta_2 \tilde{f}_2 \\
\beta_4 \tilde{f}_4 \\
\vdots \\
\beta_N \tilde{f}_N \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
-1 & -1 & -1 & \ldots & -1 \\
\alpha_1 & \alpha_3 & \alpha_5 & \alpha_7 & \\
\alpha_3 & \alpha_5 & \alpha_7 & \ddots & \\
\alpha_{N-5} & \alpha_{N-3} & \alpha_{N-1} & \ddots & \\
\alpha_{N-3} & \alpha_{N-1} & & & \\
\end{bmatrix}
\begin{bmatrix}
\tilde{\varphi}_1 \\
\tilde{\varphi}_3 \\
\tilde{\varphi}_5 \\
\vdots \\
\tilde{\varphi}_N \\
\end{bmatrix}
= 
\begin{bmatrix}
\frac{1}{2}(b - a) \\
\beta_3 \tilde{f}_3 \\
\beta_5 \tilde{f}_5 \\
\vdots \\
\beta_{N-1} \tilde{f}_{N-1} \\
\end{bmatrix}
\]

Note in the example above that, when the system decouples into two separate sub-systems, the right hand side of the boundary conditions must also account for the decoupling. For Dirichlet boundary conditions like in the example we have $\sum_j \tilde{\varphi}_j = a$ and $\sum_j \tilde{\varphi}_j(-1)^j = b$. Adding these together yields the even part $\sum_j \text{even} \tilde{\varphi}_j = (a + b)/2$. Furthermore by subtracting the latter from the former we get the odd part: $\sum_j \text{odd} \tilde{\varphi}_j = (b - a)/2$. 
4.2. Temporal and spatial discretizations

Remark 4.2. The Chebyshev-tau method is only efficient for constant coefficient equations, i.e., if the $\lambda$ coefficient in (4.35) is constant (or in our real problems the $\lambda^m_k$ coefficient, which is constant for each $k$ and $m$). For a non-constant $\lambda$ the system obtained will not be quasi tridiagonal. If a LES eddy-viscosity model is used together with the Chebyshev-tau method it cannot in practice be treated in an implicit way, since it will make $\lambda$ space dependent.

4.2.4. Computation of explicitly treated terms – Pseudospectral approximations

The right hand sides of the second order systems (4.31)–(4.33) include all the parts of the equations that are treated explicitly in time, i.e., based on the previous time-step (more precisely the previous Runge–Kutta sub-step) solution. These include different combinations of the term $H_k(u, u) = u \times \omega - f$ which include the nonlinear term and external body forces which may include the divergence of the LES SGS tensor.

A pseudo-spectral method based on a fast fourier transform (FFT) is used to compute these terms. In the Fourier–transformed horizontal directions, an original FFT is performed; and for the vertical Chebyshev direction a similar cosine FFT transform is applied. An overview how these are computed in our code is presented below.

The following procedure is adopted for the nonlinear advection term $u \times \omega$. The solution from the previous time-step is in Fourier-transformed quantities. Anti-aliasing is used through zero-padding.

1. Add zero-padding and do inverse FFT: $\hat{u}_{0\text{-padded}}, \hat{\omega}_{0\text{-padded}} \xrightarrow{F^{-1}} u, \omega$;
2. Compute $u \times \omega$;
3. Forward FFT: $u \times \omega \xrightarrow{F} \hat{u} \times \hat{\omega}$.

Thus, for the nonlinear term the steps are rather few; aside from the FFTs there are very few operations that are evaluated in physical space.

However, in case of an eddy-viscosity model it gets more complex and more computational costly. Our code follows (roughly) the following steps to compute $\mathcal{F}\{\nabla \cdot (l_s |\nabla^s u| \nabla^s u)\}$. We start in Fourier space.

1. Compute $\nabla u$ directly in Fourier space. The wall normal derivatives are found from the vorticity quantities that are stored.
2. Inverse FFT: $\nabla u \xrightarrow{F^{-1}} \nabla u$;
3. Compute $T^{SGS} = \nabla \cdot (l_s |\nabla^s u| \nabla^s u)$;
4. Forward FFT: $T^{SGS} \xrightarrow{F} \hat{T}^{SGS}$;
5. Forward Chebyshev transform: $\hat{T}^{SGS} \xrightarrow{c} \tilde{T}^{SGS}$;
6. Compute $\tilde{T}^{SGS}(1)$ and the horizontal derivatives by direct multiplication (Fourier) to obtain $\nabla \cdot \tilde{T}^{SGS}$.

7. Backward Chebyshev transform: $\nabla \cdot \tilde{T}^{SGS} \rightarrow \nabla \cdot \tilde{T}^{SGS}$.

A LES with an eddy-viscosity model must evaluate all the transforms and steps explained above whereas a DNS must only compute the nonlinear term. In Figure 4.1 the average time per time-step of typical channel flow simulations of three different resolutions are presented. As we can note, for our code, using a Smagorinsky model is approximately twice as expensive as to perform a DNS of the same resolution. We also had the chance of testing out a dynamic Smagorinsky model that furthermore is approximately twice as expensive as the standard Smagorinsky model. Moreover, the relative time spent on the explicit term for the different methods against the full computation time are presented in Table 4.1. It is clear that the computations of the explicit terms are indeed the most expensive parts of the code.

![Figure 4.1: Timing of typical Channel flow simulations.](image-url)

<table>
<thead>
<tr>
<th>DNS</th>
<th>Smagorinsky</th>
<th>Dynamic Smagorinsky</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.554</td>
<td>0.811</td>
<td>0.885</td>
</tr>
</tbody>
</table>

Table 4.1: Relative times for the explicit part of a $128^2 \times 129$ simulation.
4.2. Temporal and spatial discretizations

4.2.4.1. Anti-aliasing

A pseudo-spectral approximation does generate aliasing errors in the highest wavenumber quantities. These can be removed by several techniques, where a simple and widely used one is by adding zeros in the Fourier domain (zero-padding). The so-called 3/2 rule (Orszag 1971) is applied in the computation of the nonlinear term, where the number of grid points is increased to 3/2 of the original size with the inclusion of zeros. However, no anti-aliasing is used for the LES term in the current version of the code. An addition of anti-aliasing to the LES part by zero-padding would increase the computational cost further.

4.2.5. Notes about numerical stability

A time-step restriction due to the explicit time discretization will be present that can be more or less severe. In a DNS where the only term treated explicitly is the advection term, the time-step restriction can be approximated as a Courant–Friedrichs–Lewy (CFL) condition which is direct relation between the time-step size and the spatial resolution. The CFL criteria is limited by the smallest spatial grid spacing, which for the Fourier–Chebyshev method becomes:

\[
(\delta x)_{\text{min}} := \min \left\{ \frac{L_1}{N_1}, \frac{L_2}{N_2}, h \left(1 - \cos \left(\frac{\pi}{N_3}\right)\right) \right\}. \tag{4.43}
\]

The CFL condition is,

\[
\delta t < \frac{\alpha(\delta x)_{\text{min}}}{U_{\infty}} \tag{4.44}
\]

where \(U_{\infty}\) is here some characteristic velocity quantity, e.g. the free-stream velocity in a boundary layer, and \(\alpha\) is a parameter that depends on the time-discretization method used; it is for instance \(\sqrt{3}\) for an third order Runge–Kutta method. Following Dubois et al. (1999) the smallest Chebyshev grid spacing \((\delta x)_{\text{min},3} = h(1 - \cos(\pi/N_3))\) can be bounded as follows

\[
\frac{h}{2} \left(\frac{\pi}{N_3}\right)^2 \geq (\delta x)_{\text{min},3} \geq h \frac{\sqrt{3}}{4} \left(\frac{\pi}{N_3}\right)^2, \text{ for } N_3 \geq 6. \tag{4.45}
\]

Thus, (4.44) can be rewritten as

\[
\delta t \leq \begin{cases} \frac{\alpha L_j}{U_{\infty} N_j}, & \text{if } (\delta x)_{\text{min}} = (\delta x)_{\text{min},j}, \ j = 1, 2, \\ \frac{\alpha h \pi^2}{2 N_3^2 U_{\infty}}, & \text{if } (\delta x)_{\text{min}} = (\delta x)_{\text{min},3} \end{cases} \tag{4.46}
\]

where in most cases the lower inequality will apply due to the clustering of the Chebyshev–Gauss–Lobatto points. The CFL condition above represents the case when \(Re \to \infty\). Lundbladh et al. (1999) furthermore showed that the implicit term has a stabilizing effect on the CFL stability constraint. So we can expect (4.46) to be the worst case scenario for a DNS.
4. Numerical method

4.2.5.1. Eddy viscosity model and time step restrictions

If an eddy-viscosity model is used it is necessarily treated with the explicit time discretization scheme for Chebyshev-tau method; see remark 4.2. Unfortunately, compared to the DNS case the stability restrictions now become much more severe. A second order Chebyshev differential operator in the vertical direction typically has a largest eigenvalue that grows as $O(N_x^4)$; see Canuto et al. (1988). This essentially means that, as the number of grid points in the wall normal direction is increased, the time-step required for the explicit Runge–Kutta scheme to stay inside its stability bounds becomes very small. Citing (Canuto et al. 1988, p. 213): “An explicit time-discretization of the viscous term is possible, although rarely practical for realistic viscosities and grids. The explicit viscous stability limit scales as $1/N_x^2$ in $x$ and $1/N_y^4$ in $y$ (see Chap. 4), where $N_x$ and $N_y$ are the number of modes in the $x$ and $y$ directions respectively. The latter restriction is the most severe and virtually mandates an implicit treatment of the normal diffusion term”. With viscosity they here mean a total time and space varying viscosity ($\nu + \nu_t(x,t)$). They consider the two dimensional case with Fourier series in $x$ and Chebyshev series in $y$.

For small Reynolds numbers the stabilizing effect by the viscous term will surely also help for a LES, but not in large Reynolds numbers cases.

4.3. Boundary condition implementation

Boundary conditions can be imposed through the framework of homogeneous and particular solutions using the transformations (4.10)–(4.11) back and forth from normal-velocity normal-vorticity to the horizontal velocity quantities. In this section we present a newly tested implementation in which arbitrary linear, so far first order, boundary conditions can be imposed. These can be of either Dirichlet, Neumann or Robin type. This is an extension to the previous work by e.g. Kim et al. (1987) and other channel flow codes where only simple no-slip boundary conditions are imposed.

4.3.1. General boundary condition systems

In order to solve the Navier–Stokes problem (4.1) we need to impose boundary conditions on $u$. The Fourier transformed boundary conditions can be defined as

$$ B_j^{-} \hat{u}_j^-(k) = B_j^{+} \hat{u}_j^+(k) = B_{0,j}^{-} \hat{u}_j^- (0) = B_{0,j}^{+} \hat{u}_j^+ (0) = 0, \quad j = 1, 2, 3, \quad (4.47) $$

where $B_j^\pm, B_{0,j}^\pm$ are linear boundary operators for $k \in S_N \setminus 0$ and $k = 0$ respectively and $\hat{u}_j^-(k) := \hat{u}_j^{n,m}(k,-1)$ and $\hat{u}_j^+(k) := \hat{u}_j^{n,m}(k,1)$ the velocity quantities at the boundaries. The superscripts $\pm$ denote $x_3$ on $\{-1,1\}$ and the time-step indices have been dropped for the sake of simplicity.

4.3.1.1. Non-zero wavenumbers

For $k \in S_N \setminus 0$ the fourth order equation for normal velocity (4.12b) require four boundary conditions to be well posed and the second order equation for
the normal vorticity (4.12a) requires two. Thus, the general solutions can be written as follow

$$\begin{align*}
\hat{u}_{3}^{n,m} &= \hat{u}_{3,p}^{n,m} + \sum_{l=1}^{4} c_{l}^{u} \hat{u}_{3,h_{l}}, & (k, x_{3}) \in S_{N} \setminus 0 \times [-1, 1] \tag{4.48a} \\
\hat{\omega}_{3}^{n,m} &= \hat{\omega}_{3,p}^{n,m} + \sum_{l=1}^{2} c_{l}^{\omega} \hat{\omega}_{3,h_{l}}, & (k, x_{3}) \in S_{N} \setminus 0 \times [-1, 1] \tag{4.48b}
\end{align*}$$

where the subscript $p$ denotes particular- and $h_{l}$ homogeneous solution. In order to find an unique solution for $\hat{u}_{3,m}^{n}$ and $\hat{\omega}_{3,m}^{n}$ we need to determine the unknown coefficients $c_{1}^{u}, c_{2}^{u}, c_{3}^{u}, c_{4}^{u}, c_{1}^{\omega},$ and $c_{2}^{\omega}$. We need to impose four boundary conditions on $\hat{u}_{3,m}^{n}$ and two on $\hat{\omega}_{3,m}^{n}$. However, since the homogeneous and particular solutions for $\hat{u}_{3,m}^{n}$ and $\hat{\omega}_{3,m}^{n}$ are known we can use the transformations (4.10)–(4.11) to solve for coefficients corresponding to the appropriate boundary conditions on $\hat{u}$.

In the transformation of homogeneous solutions we can whenever possible use trivial homogeneous solutions (the constant zero solution). The first four homogeneous solutions are found from $(\hat{u}_{3,h_{l}}, 0) \mapsto (\hat{u}_{1,h_{l}}, \hat{u}_{2,h_{l}})$, $l = 1, 2, \ldots, 4$ and the fifth and sixth from $(0, \hat{\omega}_{3,h_{l}}) \mapsto (\hat{u}_{1,h_{l}}, \hat{u}_{2,h_{l}})$, $l = 5, 6$. For the particular solutions there are no trivial solutions but on the other hand only six transformations needed; one per boundary condition: $(\hat{u}_{3,p}, \hat{\omega}_{3,p}) \mapsto (\hat{u}_{1,p}, \hat{u}_{2,p})$. These are moved to the right hand side of the equations. Thus, assuming linear boundary condition operators we solve, for each $k \in S_{N} \setminus 0$ a linear system $A_{k}c_{k} = b_{k}$ with

$$A_{k} = \begin{bmatrix}
B_{1}^{+} \hat{u}_{1,h_{1}} & B_{1}^{-} \hat{u}_{1,h_{2}} & B_{1}^{-} \hat{u}_{1,h_{3}} & B_{1}^{-} \hat{u}_{1,h_{4}} & B_{1}^{-} \hat{u}_{1,h_{5}} & B_{1}^{-} \hat{u}_{1,h_{6}} \\
B_{2}^{+} \hat{u}_{2,h_{1}} & B_{2}^{-} \hat{u}_{2,h_{2}} & B_{2}^{-} \hat{u}_{2,h_{3}} & B_{2}^{-} \hat{u}_{2,h_{4}} & B_{2}^{-} \hat{u}_{2,h_{5}} & B_{2}^{-} \hat{u}_{2,h_{6}} \\
B_{3}^{+} \hat{u}_{3,h_{1}} & B_{3}^{-} \hat{u}_{3,h_{2}} & B_{3}^{-} \hat{u}_{3,h_{3}} & B_{3}^{-} \hat{u}_{3,h_{4}} & 0 & 0 \\
B_{4}^{+} \hat{u}_{1,h_{1}} & B_{4}^{+} \hat{u}_{1,h_{2}} & B_{4}^{+} \hat{u}_{1,h_{3}} & B_{4}^{+} \hat{u}_{1,h_{4}} & B_{4}^{+} \hat{u}_{1,h_{5}} & B_{4}^{+} \hat{u}_{1,h_{6}} \\
B_{5}^{+} \hat{u}_{2,h_{1}} & B_{5}^{+} \hat{u}_{2,h_{2}} & B_{5}^{+} \hat{u}_{2,h_{3}} & B_{5}^{+} \hat{u}_{2,h_{4}} & B_{5}^{+} \hat{u}_{2,h_{5}} & B_{5}^{+} \hat{u}_{2,h_{6}} \\
B_{6}^{+} \hat{u}_{3,h_{1}} & B_{6}^{+} \hat{u}_{3,h_{2}} & B_{6}^{+} \hat{u}_{3,h_{3}} & B_{6}^{+} \hat{u}_{3,h_{4}} & 0 & 0
\end{bmatrix}, \tag{4.49}
$$

$$b_{k} = \begin{bmatrix}
B_{1}^{+} \hat{u}_{1}^{+} - B_{1}^{-} \hat{u}_{1}^{-} \\
B_{2}^{+} \hat{u}_{2}^{+} - B_{2}^{-} \hat{u}_{2}^{-} \\
B_{3}^{+} \hat{u}_{3}^{+} - B_{3}^{-} \hat{u}_{3}^{-} \\
B_{4}^{+} \hat{u}_{1}^{+} - B_{4}^{-} \hat{u}_{1}^{-} \\
B_{5}^{+} \hat{u}_{2}^{+} - B_{5}^{-} \hat{u}_{2}^{-} \\
B_{6}^{+} \hat{u}_{3}^{+} - B_{6}^{-} \hat{u}_{3}^{-}
\end{bmatrix}, \tag{4.50}
$$

$$c_{k} = (c_{1}^{u}, c_{2}^{u}, c_{3}^{u}, c_{4}^{u}, c_{1}^{\omega}, c_{2}^{\omega})^{	op}. \tag{4.51}$$
where the transformations for the horizontal velocities are given by

\[
B^-_{1, h_l} u^-_{1, h_l} = \begin{cases} 
  iK_1 |K|^2 \frac{d\hat{u}_{3, h_l}}{dx_3}, & l = 1, 2, \ldots, 4 \\
  -iK_2 |K|^2 \frac{d\hat{\omega}_{3, h_l}}{dx_3}, & l = 5, 6 
\end{cases} 
\]

\[
B^-_{2, h_l} u^-_{2, h_l} = \begin{cases} 
  iK_2 |K|^2 \frac{d\hat{u}_{3, h_l}}{dx_3}, & l = 1, 2, \ldots, 4 \\
  -iK_1 |K|^2 \frac{d\hat{\omega}_{3, h_l}}{dx_3}, & l = 5, 6 
\end{cases} 
\]

\[
B^+_{1, h_l} u^+_{1, h_l} = \begin{cases} 
  iK_1 |K|^2 \frac{d\hat{u}_{3, h_l}}{dx_3}, & l = 1, 2, \ldots, 4 \\
  -iK_2 |K|^2 \frac{d\hat{\omega}_{3, h_l}}{dx_3}, & l = 5, 6 
\end{cases} 
\]

\[
B^+_{2, h_l} u^+_{2, h_l} = \begin{cases} 
  iK_2 |K|^2 \frac{d\hat{u}_{3, h_l}}{dx_3}, & l = 1, 2, \ldots, 4 \\
  -iK_1 |K|^2 \frac{d\hat{\omega}_{3, h_l}}{dx_3}, & l = 5, 6 
\end{cases} 
\]

and

\[
B^-_{1, h_l} \hat{u}^-_{1, p} = \frac{i}{|K|^2} \left( K_1 B^-_{1} \frac{d\hat{u}_{3, p}}{dx_3} - K_2 B^-_{1} \frac{d\hat{\omega}_{3, p}}{dx_3} \right) 
\]

\[
B^-_{2, h_l} \hat{u}^-_{2, p} = \frac{i}{|K|^2} \left( K_2 B^-_{2} \frac{d\hat{u}_{3, p}}{dx_3} + K_1 B^-_{2} \frac{d\hat{\omega}_{3, p}}{dx_3} \right) 
\]

\[
B^+_{1, h_l} \hat{u}^+_{1, p} = \frac{i}{|K|^2} \left( K_1 B^+_{1} \frac{d\hat{u}_{3, p}}{dx_3} - K_2 B^+_{1} \frac{d\hat{\omega}_{3, p}}{dx_3} \right) 
\]

\[
B^+_{2, h_l} \hat{u}^+_{2, p} = \frac{i}{|K|^2} \left( K_2 B^+_{2} \frac{d\hat{u}_{3, p}}{dx_3} + K_1 B^+_{2} \frac{d\hat{\omega}_{3, p}}{dx_3} \right) . 
\]

4.3.1.2. Zero wavenumbers

For \( k = 0 \) there are two boundary conditions per horizontal velocity quantity that each yields one second order system. Since there are two individual systems solving similar equations the same homogeneous solutions can be used for both. We have

\[
\hat{u}^{n,m}_j = \hat{u}^{n,m}_{1,p} + \sum_{l=1}^{2} \delta_{j,l} \hat{v}^{n,m}_{h_l}, \quad j = 1, 2, \quad (k, x_3) \in \{0\} \times [-1, 1], 
\]

where \( \hat{v}^{n,m}_{h_l} = \hat{u}^{n,m}_{1,h_l} = \hat{u}^{n,m}_{2,h_l}, \quad l = 1, 2. \) Furthermore we define like-wise to the non-zero wavenumber case \( \hat{v}^{\pm}_{h_l} := \hat{v}^{m,n}_{h_l}(0, \pm 1) \) and \( \hat{v}^{\pm}_{p} := v^{m,n}_{p}(0, \pm 1). \) Two
boundary condition systems can now be stated as $A_0^{(j)} c_0^{(j)} = b_0^{(j)}$, $j = 1, 2$, with

$$A_0^{(j)} := \begin{bmatrix} B_{0,j}^- \hat{v}_{h_1}^- & B_{0,j}^- \hat{v}_{h_2}^- \\ B_{0,j}^+ \hat{v}_{h_1}^+ & B_{0,j}^+ \hat{v}_{h_2}^+ \end{bmatrix}, \quad j = 1, 2,$$

(4.61)

$$b_0^{(j)} := \begin{pmatrix} B_{0,j}^- \hat{u}_j^- - B_{0,j}^- \hat{u}_{p,j}^- \\ B_{0,j}^+ \hat{u}_j^+ - B_{0,j}^+ \hat{u}_{p,j}^+ \end{pmatrix}, \quad j = 1, 2,$$

(4.62)

$$c_0^{(j)} := (c_{j,1}^0, c_{j,2}^0)^T, \quad j = 1, 2.$$

(4.63)

### 4.3.1.3. Examples

Two examples illustrating how the boundary condition systems are built up for different boundary conditions are presented below. Example 4.2 is a typical example showing horizontally inhomogeneous boundary conditions, and Example 4.3 shows the system used for the wall modeled open channel flow simulations presented in §5.3.

**Example 4.2 (Dirichlet boundary conditions).** Suppose we want to impose the following inhomogeneous Dirichlet boundary conditions:

$$\begin{align*}
&\begin{cases}
  u_1 = f(x_1, x_2), & u_2 = g(x_1, x_2), & u_3 = 0, & \text{on } x_3 = -1, \\
  u_1 = a, & u_2 = b, & u_3 = 0, & \text{on } x_3 = 1.
\end{cases}
\end{align*}$$

In Fourier space and using the $\pm$ notation for the upper and lower boundaries these are equivalent to

$$\begin{align*}
&\begin{cases}
  \hat{u}_1^- = \hat{f}_k, & \hat{u}_2^- = \hat{g}_k, & \hat{u}_3^- = 0, \\
  \hat{u}_1^+ = 0, & \hat{u}_2^+ = 0, & \hat{u}_3^+ = 0
\end{cases}, \quad k \in S_N \setminus 0, \\
&\begin{cases}
  \hat{u}_1^- = \hat{f}_0, & \hat{u}_2^- = \hat{g}_0, & \hat{u}_3^- = 0, \\
  \hat{u}_1^+ = a, & \hat{u}_2^+ = b, & \hat{u}_3^+ = 0
\end{cases}, \quad k = 0.
\end{align*}$$
The linear systems that are used to solve the $c_k$ and $c_0^{(j)}$ coefficients here become

$$A_k = \begin{bmatrix}
\hat{u}_{1,h_1}^- & \hat{u}_{1,h_2}^- & \hat{u}_{1,h_3}^- & \hat{u}_{1,h_4}^- & \hat{u}_{1,h_5}^- & \hat{u}_{1,h_6}^- \\
\hat{u}_{2,h_1}^- & \hat{u}_{2,h_2}^- & \hat{u}_{2,h_3}^- & \hat{u}_{2,h_4}^- & \hat{u}_{2,h_5}^- & \hat{u}_{2,h_6}^- \\
\hat{u}_{3,h_1}^- & \hat{u}_{3,h_2}^- & \hat{u}_{3,h_3}^- & \hat{u}_{3,h_4}^- & 0 & 0 \\
\hat{u}_{1,h_1}^+ & \hat{u}_{1,h_2}^+ & \hat{u}_{1,h_3}^+ & \hat{u}_{1,h_4}^+ & \hat{u}_{1,h_5}^+ & \hat{u}_{1,h_6}^+ \\
\hat{u}_{2,h_1}^+ & \hat{u}_{2,h_2}^+ & \hat{u}_{2,h_3}^+ & \hat{u}_{2,h_4}^+ & \hat{u}_{2,h_5}^+ & \hat{u}_{2,h_6}^+ \\
\hat{u}_{3,h_1}^+ & \hat{u}_{3,h_2}^+ & \hat{u}_{3,h_3}^+ & \hat{u}_{3,h_4}^+ & 0 & 0
\end{bmatrix},$$

$$b_k = \begin{bmatrix}
\hat{f}_k - \hat{u}_{1,p}^- \\
\hat{g}_k - \hat{u}_{2,p}^- \\
-\hat{u}_{3,p}^- \\
-\hat{u}_{1,p}^+ \\
-\hat{u}_{2,p}^+ \\
-\hat{u}_{3,p}^+
\end{bmatrix},$$

$$A_0^{(1)} = A_0^{(2)} = \begin{bmatrix}
\hat{v}_{h_1}^- & \hat{v}_{h_2}^- \\
\hat{v}_{h_1}^+ & \hat{v}_{h_2}^+
\end{bmatrix},$$

$$b_0^{(1)} = \left( \begin{array}{c}
\hat{f}_0 - \hat{u}_{p,1}^- \\
\hat{g}_0 - \hat{u}_{p,2}^-
\end{array} \right), \quad b_0^{(2)} = \left( \begin{array}{c}
\hat{f}_0 - \hat{u}_{p,2}^- \\
\hat{g}_0 - \hat{u}_{p,2}^+
\end{array} \right).$$

**Example 4.3 (Robin/Neumann boundary conditions).** Suppose we want to impose constant coefficient partial slip and no penetration boundary conditions on the lower boundary and free-slip (homogeneous Neumann) and no penetration on the upper. In physical space these reads:

$$\begin{cases}
 u_3 = 0, & \beta_j u_j + \frac{\partial u_j}{\partial x_3} = 0, & j = 1, 2 & \text{on } x_3 = -1, \\
 u_3 = 0, & \frac{\partial u_j}{\partial x_3} = 0, & j = 1, 2 & \text{on } x_3 = 1.
\end{cases}$$

In Fourier space ($x_3$ derivative unaffected) these are simply equivalent to

$$\begin{cases}
 \hat{u}_3^- = 0, & \beta_j \hat{u}_j^- + \partial_{x_3} \hat{u}_j^- = 0, & j = 1, 2, \\
 \hat{u}_3^+ = 0, & \beta_j \hat{u}_j^+ = 0, & j = 1, 2, \\
\end{cases} \quad \forall k \in S_N.$$
The homogeneous and particular solutions used to build the general solutions are arbitrary in the sense that we can choose boundary conditions arbitrarily when we solve the second order systems. To be as universal as possible but also for simplicity we use Dirichlet boundary conditions for all homogeneous and particular solutions. For the boundary values we use, for simplicity, different combinations of 0 and 1 in all cases.

\[ A_k = \begin{bmatrix}
\beta_1 \hat{u}_{1,h_1} + \partial_3 \hat{u}_{1,h_1} & \ldots & \beta_1 \hat{u}_{1,h_4} + \partial_3 \hat{u}_{1,h_4} & \beta_1 \hat{u}_{1,h_5} + \partial_3 \hat{u}_{1,h_5} \\
\beta_2 \hat{u}_{2,h_1} + \partial_3 \hat{u}_{2,h_1} & \ldots & \beta_2 \hat{u}_{2,h_4} + \partial_3 \hat{u}_{2,h_4} & \beta_2 \hat{u}_{2,h_5} + \partial_3 \hat{u}_{2,h_5} \\
\hat{u}_{3,h_1} & \ldots & \hat{u}_{3,h_4} & 0 & 0 \\
\partial_3 \hat{u}_{1,h_1} & \ldots & \partial_3 \hat{u}_{1,h_4} & \beta_3 \hat{u}_{1,h_5} & \beta_3 \hat{u}_{1,h_6} \\
\partial_3 \hat{u}_{2,h_1} & \ldots & \partial_3 \hat{u}_{2,h_4} & \beta_3 \hat{u}_{2,h_5} & \beta_3 \hat{u}_{2,h_6} \\
\hat{u}_{3,h_1} & \ldots & \hat{u}_{3,h_4} & 0 & 0
\end{bmatrix}, \]

\[ b_k = \begin{bmatrix}
-(\beta_1 \hat{u}_{1,p} + \partial_3 \hat{u}_{1,p}) \\
-(\beta_2 \hat{u}_{2,p} + \partial_3 \hat{u}_{2,p}) \\
-\hat{u}_{3,p} \\
-\partial_3 \hat{u}_{1,p} \\
-\partial_3 \hat{u}_{2,p} \\
-\hat{u}_{3,p}
\end{bmatrix}, \]

\[ A_0^{(1)} = \begin{bmatrix}
\beta_1 \hat{v}_{h_1} + \partial_3 \hat{v}_{h_1} & \beta_1 \hat{v}_{h_2} + \partial_3 \hat{v}_{h_2} \\
\partial_3 \hat{v}_{h_1} & \partial_3 \hat{v}_{h_2}
\end{bmatrix}, \quad A_0^{(2)} = \begin{bmatrix}
\beta_2 \hat{v}_{h_1} + \partial_3 \hat{v}_{h_1} & \beta_2 \hat{v}_{h_2} + \partial_3 \hat{v}_{h_2} \\
\partial_3 \hat{v}_{h_1} & \partial_3 \hat{v}_{h_2}
\end{bmatrix}, \]

\[ b_0^{(1)} = \begin{bmatrix}
-(\beta_1 \hat{u}_{p,1} + \partial_3 \hat{u}_{p,1}) \\
-\partial_3 \hat{u}_{p,1}
\end{bmatrix}, \quad b_0^{(2)} = \begin{bmatrix}
-(\beta_1 \hat{u}_{p,2} + \partial_3 \hat{u}_{p,2}) \\
-\partial_3 \hat{u}_{p,2}
\end{bmatrix}. \]

As is clearly seen in Example 4.3, imposing different friction coefficients for different wavenumbers (as discussed in §3.3.3) is simply done by editing \( \beta_1 \) and \( \beta_2 \) for different \( k \) since the method solves for each wavenumber individually.

### 4.3.2. Solving for homogeneous and particular equations

The homogeneous and particular solutions used to build the general solutions are solved for by the Chebyshev-tau method, as explained in §4.2.3.2. These solutions are arbitrary in the sense that we can choose boundary conditions arbitrary when we solve the second order systems. To be as universal as possible but also for simplicity we use Dirichlet boundary conditions for all homogeneous and particular solutions. For the boundary values we use, for simplicity, different combinations of 0 and 1 in all cases.
4. Numerical method

4.3.2.1. Non-zero wavenumbers

For the non-zero wavenumbers $\mathbf{k} \in S_N \setminus \mathbf{0}$ the homogeneous solutions for the normal velocity are computed in two steps due to the splitting of the fourth order equation. First, homogeneous solutions for the auxiliary variable $\phi$ are computed. These are obtained from

\[
\begin{aligned}
\left\{ \left( \frac{d^2}{dx_3^2} - \lambda_k^m \right) \phi_{h_l}(\mathbf{k},x_3) = 0, \quad l = 1, \ldots, 4, \quad -1 < x_3 < 1, \right. \\
\phi_{h_1}(\mathbf{k}, -1) = 0, \quad \phi_{h_1}(\mathbf{k}, 1) = 0, \\
\phi_{h_2}(\mathbf{k}, -1) = 0, \quad \phi_{h_2}(\mathbf{k}, 1) = 0, \\
\phi_{h_3}(\mathbf{k}, -1) = 1, \quad \phi_{h_3}(\mathbf{k}, 1) = 0, \\
\phi_{h_4}(\mathbf{k}, -1) = 0, \quad \phi_{h_4}(\mathbf{k}, 1) = 1,
\end{aligned}
\]  

(4.64)

Where the first and second solutions are simply chosen as the trivial solution $\phi_{h_1}^{n,m}(\mathbf{k},x_3) = \phi_{h_2}^{n,m}(\mathbf{k},x_3) = 0$. The homogeneous solutions for $\hat{u}_3$ can now be obtained by solving

\[
\begin{aligned}
\left\{ \left( \frac{d^2}{dx_3^2} - |\mathbf{K}|^2 \right) \hat{u}_{3,h_l}^{n,m}(\mathbf{k},x_3) = \phi_{h_l}^{n,j}(\mathbf{k},x_3), \quad l = 1, \ldots, 4, \quad -1 < x_3 < 1, \right. \\
\hat{u}_{3,h_1}^{n,m}(\mathbf{k}, -1) = 1, \quad \hat{u}_{3,h_1}^{n,m}(\mathbf{k}, 1) = 0, \\
\hat{u}_{3,h_2}^{n,m}(\mathbf{k}, -1) = 0, \quad \hat{u}_{3,h_2}^{n,m}(\mathbf{k}, 1) = 1, \\
\hat{u}_{3,h_3}^{n,m}(\mathbf{k}, -1) = 0, \quad \hat{u}_{3,h_3}^{n,m}(\mathbf{k}, 1) = 0, \\
\hat{u}_{3,h_4}^{n,m}(\mathbf{k}, -1) = 0, \quad \hat{u}_{3,h_4}^{n,m}(\mathbf{k}, 1) = 0,
\end{aligned}
\]  

(4.65)

Moreover, the homogeneous solutions for the normal vorticity are solved from

\[
\begin{aligned}
\left\{ \left( \frac{d^2}{dx_3^2} - \lambda_k^m \right) \hat{\omega}_{3,h_l}^{n,m}(\mathbf{k},x_3) = 0, \quad l = 1, 2, \quad -1 < x_3 < 1, \right. \\
\hat{\omega}_{3,h_1}^{n,m}(\mathbf{k}, -1) = 1, \quad \hat{\omega}_{3,h_1}^{n,m}(\mathbf{k}, 1) = 0, \\
\hat{\omega}_{3,h_2}^{n,m}(\mathbf{k}, -1) = 0, \quad \hat{\omega}_{3,h_2}^{n,m}(\mathbf{k}, 1) = 1.
\end{aligned}
\]  

(4.66)
The particular solutions for the zero wavenumbers are furthermore solved from

\[
\begin{align*}
\left\{ \left( \frac{d^2}{dx_3^2} - \lambda^m_k \right) \omega^{n,m}_{3,p}(k, x_3) = F^{n,m-1}_k, \quad -1 < x_3 < 1, \right. \\
\omega^{n,m}_{3,p}(k, \pm1) = 0. \\
\end{align*}
\]

(4.67)

\[
\begin{align*}
\left\{ \left( \frac{d^2}{dx_3^2} - \lambda^m_k \right) \phi_p(k, x_3) = G^{n,m-1}_k, \quad -1 < x_3 < 1, \right. \\
\phi_p(k, \pm1) = 0. \\
\end{align*}
\]

(4.68)

\[
\begin{align*}
\left\{ \left( \frac{d^2}{dx_3^2} - |K|^2 \right) \hat{u}^{n,m}_{3,p}(k, x_3) = \phi_p(k, x_3), \quad -1 < x_3 < 1, \right. \\
\hat{u}^{n,m}_{3,p}(k, \pm1) = 0. \\
\end{align*}
\]

(4.69)

4.3.2.2. Zero wavenumbers

For \(k = 0\) the homogeneous solutions are solved from:

\[
\begin{align*}
\left\{ \left( \frac{d^2}{dx_3^2} - \lambda^0_0 \right) v^{n,m}_{j,h_l}(x_3) = 0, \quad l = 1, 2, \quad j = 1, 2, \quad -1 < x_3 < 1, \\
v^{n,m}_{j,h_1}(-1) = 1, \quad v^{n,m}_{j,h_1}(1) = 0, \\
v^{n,m}_{j,h_2}(-1) = 0, \quad v^{n,m}_{j,h_2}(1) = 1. \\
\end{align*}
\]

(4.70)

And particular solutions from:

\[
\begin{align*}
\left\{ \left( \frac{d^2}{dx_3^2} - \lambda^0_0 \right) \hat{u}^{n,m}_{j,p}(0, x_3) = H^{n,m-1}_{0,j}, \quad j = 1, 2, \quad -1 < x_3 < 1, \\
\hat{u}^{n,m}_{j,p}(0, \pm1) = 0, \quad j = 1, 2. \\
\end{align*}
\]

(4.71)

4.3.3. Notes regarding the accuracy of the boundary condition systems

The boundary conditions for the homogeneous solutions can be chosen with the boundary condition matrices in mind. For instance, we usually employ Dirichlet boundary conditions for \(u_3\) for which the rows in the boundary condition matrices become the boundary conditions chosen to solve for the homogeneous solutions, i.e. \(\{1, 0, 0, 0, 0, 0\}\) for the \(u_3^-\) row, and \(\{0, 1, 0, 0, 0, 0\}\) for the \(u_3^+\) row respectively. Furthermore, a Neumann condition for the horizontal quantities \(u_1\) and \(u_2\) yield the rows becomes similar to the boundary conditions for \(\phi_{h_i}\), i.e., due to the second derivative that appears in the transformation (e.g. a \(B^{-1} = d/dx_3\) in equation 4.52). However, a fully diagonal matrix is hard to obtain due to the remaining rows that depend on the boundary conditions on \(\omega_3\). Also, the matrices may change from case to case; just look at the matrices for the two examples 4.2–4.3.

The condition number of a matrix \(A \in \mathbb{R}^{M \times N}\) is defined as \(\kappa(A) := \|A\|_\infty \|A^{-1}\|_\infty\) where \(\|A\|_\infty = \max_{1 \leq i \leq M} \sum_{j=1}^{N} |(A)_{ij}|\) is the infinite matrix
norm that basically gives the value of the largest element in the matrix. A matrix with a large variation between its smallest and largest values gives a large condition number. The condition number can be seen as a measure of the sensibility of the linear system to small variations in the data. More practically it becomes a measure on the sensibility of the system to round off errors. A condition number of $10^k$ leads roughly to a loss of $k$ significant digits in the final solution.

The size and variability of the elements in the $A_k$ matrix for non-zero wavenumbers depend on the size of $K_j/|K|$, $B \frac{\partial \hat{\omega}^\pm_{3,h_1}}{\partial x_3}$ and $B \hat{\omega}^\pm_{3,h_1-4}$ where $B$ is some boundary condition operator. The size of $K_j/|K|$ typically has a rather low impact since $|K_j| \leq |K|$. However, the size of the other two would have an impact on the condition number of the matrix. Take for instance the case $B = \frac{d}{dx_3}$ and consider the $B \hat{\omega}^\pm_{3,h_1-4}$ values. We usually solve for the homogeneous solutions using Dirichlet boundary conditions (for here see equation 4.66) thus the value of the derivative at a boundary is not directly controlled. The size of the derivative can be derived analytically. We have a homogeneous Dirichlet boundary value problem on the form

$$
\begin{cases}
\left( \frac{d^2}{dx^2} - \Lambda^2 \right) \xi(x) = 0, & -1 < x < 1, \\
\xi(-1) = 1, & \xi(1) = 0,
\end{cases}
$$

has the following analytic solution

$$
\xi(x) = \left( \frac{1}{e^{4\Lambda} - 1} \right) \left( e^{\lambda(3-x)} - e^{\Lambda(x+1)} \right)
$$

At the boundaries we then have

\[
\frac{d\xi}{dx}(-1) = -\Lambda \left( \frac{e^{4\Lambda} + 1}{e^{4\Lambda} - 1} \right) \approx -\Lambda, \quad \text{as } \Lambda \gg 1,
\]

\[
\frac{d\xi}{dx}(1) = -2\Lambda \left( \frac{e^{2\Lambda}}{e^{4\Lambda} - 1} \right) \approx 0, \quad \text{as } \Lambda \gg 1,
\]

\[
\frac{d^2\xi}{dx^2}(-1) = -\Lambda^2,
\]

\[
\frac{d^2\xi}{dx^2}(1) = 0.
\]

Thus for a Neumann or Robin boundary condition where the boundary condition operators include a first derivative, the elements computed from $\hat{\omega}_3$ solutions become

$$
- \frac{iK_2}{|K|^2} \frac{\partial \hat{\omega}^-_{3,h_1-4}}{\partial x_3} \sim \frac{K_2}{|K|^2} \sqrt{\frac{\lambda_m^k}{\nu \alpha_m \delta t}} \sim \frac{K_2}{|K|^2} \sqrt{\frac{2}{\nu \alpha_m \delta t}} - |K|^2.
$$

Thus, both the Reynolds number ($\nu = 1/\text{Re}$) and the time step size $\delta t$ plays in to a higher extent. For a Dirichlet boundary condition, the same problem does
Table 4.2: Maximum condition numbers for the non-zero wavenumber boundary condition matrix, i.e., $\max_k \kappa(A_k)$.

<table>
<thead>
<tr>
<th>Resolution</th>
<th>BC type</th>
<th>Re = 10³</th>
<th>Re = 10⁴</th>
<th>Re = 10⁵</th>
</tr>
</thead>
<tbody>
<tr>
<td>64² × 65</td>
<td>Dirichlet</td>
<td>0.13 × 10⁶</td>
<td>0.83 × 10⁶</td>
<td>0.78 × 10⁷</td>
</tr>
<tr>
<td></td>
<td>Neumann</td>
<td>0.11 × 10⁶</td>
<td>0.10 × 10⁷</td>
<td>0.10 × 10⁸</td>
</tr>
<tr>
<td></td>
<td>Robin</td>
<td>0.17 × 10⁶</td>
<td>0.16 × 10⁷</td>
<td>0.16 × 10⁸</td>
</tr>
<tr>
<td>128² × 129</td>
<td>Dirichlet</td>
<td>0.24 × 10⁶</td>
<td>0.73 × 10⁶</td>
<td>0.42 × 10⁷</td>
</tr>
<tr>
<td></td>
<td>Neumann</td>
<td>0.11 × 10⁶</td>
<td>0.56 × 10⁶</td>
<td>0.50 × 10⁷</td>
</tr>
<tr>
<td></td>
<td>Robin</td>
<td>0.14 × 10⁶</td>
<td>0.71 × 10⁶</td>
<td>0.63 × 10⁷</td>
</tr>
</tbody>
</table>

appear for the $B \frac{du_{3, h}}{dx_3}$ as the homogeneous solutions for $\hat{u}_{3, h}$, are computed with Dirichlet boundary conditions.

The Reynolds number dependency on the condition number of the $A_k$ was further tested. In table 4.2 the maximum condition number for different resolutions and boundary conditions is presented. It is evident that there is a clear Reynolds number dependency. Neumann and Robin conditions for the horizontal quantities only imply slightly worse conditioned systems over a full Dirichlet case. Increasing the resolution does not change the condition number significantly. For the Neumann and Robin cases a slight improvement can be seen.

One method to overcome serious round-off errors due to the ill-conditioning of the system $A_k c_k = b_k$ would be to use high precision arithmetics. If the Reynolds number is kept at a sufficiently low level, the accuracy using double precision may be sufficient in most situations, but also quadruple precision would be an alternative for these small systems. Another alternative is to use Neumann boundary conditions when solving for homogeneous $\hat{\omega}_3$ solutions, which may directly control the size of the boundary condition values for the Neumann case. However, this should require the code to compute the homogeneous and particular solutions differently for different boundary conditions. However, for e.g. the Dirichlet case $\hat{u}_3$ where the transformations have $\frac{d\hat{u}_{3, h}}{dx_3}$ inside them it would not be possible to overcome this issue anyway.

Also, important to note is also that the condition number of the discrete Chebyshev-tau systems that we solve for the homogeneous and particular solutions typically grow with problem size; see e.g. Canuto et al. (1988). This must also be accounted for as the overall accuracy is studied.

4.4. Artificial viscosity for high Reynolds number LES

As was shown in §4.3.3, for the boundary condition systems the accuracy of the method highly depends on the size of the Reynolds number. Furthermore, the Chebyshev-tau systems may be ill-conditioned as well. Very large Reynolds
numbers are a problem that affect the numerical accuracy. For an atmospheric boundary simulation where the Reynolds numbers can be as large as $10^8 - 10^{10}$ these problems become severe. Using the normal-velocity normal-vorticity formulation the implicitly treated viscous term is important and necessary for the boundary condition implementation. The whole method relies on that term. On the other hand, as mentioned in remark 4.2, we cannot simply treat the eddy-viscosity in an implicit way; the Chebyshev-tau system matrix will not be quasi-tridiagonal anymore and the computational cost will increase substantially.

A workaround for using large Reynolds numbers in order to overcome possible ill-conditioned Chebyshev-tau systems and also to stabilize the time discretization, is to introduce an artificial viscosity $\tilde{\nu}$ that is added to the implicitly treated constant viscosity $\nu$ and subtracted from the explicitly treated eddy-viscosity $\nu_t$. This method was also applied by Karniadakis, Orszag and Yakhot (see Galperin & Orszag 1993, p. 164).

With the artificial viscosity applied the equation of motion (4.1a) is rewritten as

$$\frac{\partial u}{\partial t} + N(u) + \nabla q - (\nu + \tilde{\nu})\Delta u = 0.$$  \hspace{1cm} (4.72)

where the nonlinear term now includes an eddy-viscosity term and rewrites into

$$N(u) = \omega \times u - f - \nabla \cdot (\nu_t(x,t) - \tilde{\nu})\nabla^s u.$$  \hspace{1cm} (4.73)

Now it is possible that for instance set $\nu = 0$ which represents the case $\text{Re} \approx \infty$. Typically in the LES simulations of this thesis the artificial viscosity is chosen as $\tilde{\nu} = 0.001$. For consistency with the notation in this chapter, the bars for filtered velocities were left out.

### 4.5. Scalar equation discretization

Solving the scalar equation (2.6) with a Fourier–Chebyshev discretization is easier than solving the Navier–Stokes equations. No transformation between variables are needed like in the normal-velocity normal-vorticity formulation; the discretization is performed directly for the scalar variable. The discretization procedure follows the same steps as for the Navier–Stokes equations yielding a second order equation similar to the one for the zero wavenumber horizontal velocities (4.30) but for all wavenumbers. The boundary condition implementation is also similar that for the zero wavenumber horizontal velocities. One $2 \times 2$ system needs to be solved at each of the two vertical boundaries. Furthermore, the LES part is treated in a similar way. For the eddy-diffusivity model we also use an artificial diffusivity constant $\tilde{\kappa}$ in order to handle the large diffusivity $\kappa = 1/(\text{Re Pr})$ corresponding to a large Reynolds number case similar to what we presented in §4.4.
Chapter 5

Numerical results

In this chapter we present the results of different numerical simulations that were performed using the numerical method of chapter 4 together with the boundary condition ideas presented in chapter 3. To study the effects of different mechanisms and modeling assumptions in detail we start simple and increase the complexity in a step-wise manner. In Section 5.1 a short introduction to the flow cases of the chapter are introduced and the way we non-dimensionalize the equations are presented. In Section 5.2 we start simulating comparably low Reynolds number turbulent channel flows of $Re_\tau = 180$ and examine the effects of the partial slip boundary conditions. In Section 5.3 we perform a detailed study of the boundary conditions in a high Reynolds number open channel flow, analogous to a simplified neutral atmospheric boundary layer. Finally in Section 5.4 we present some preliminary results on low to high Reynolds number stably stratified flows.

The following non-dimensional computational domain is used in all simulations of this chapter

$$\Omega := [0, 4\pi] \times [0, 2\pi] \times [-1, 1],$$

(5.1)

where the horizontal directions are chosen divisible by $\pi$ since the Fourier expansions are $\pi$-periodic. Moreover, the vertical coordinates are chosen with the range $[-1, 1]$ of the Chebyshev basis in mind. The specific reference values for length and velocity are introduced for specific flow cases in §5.1.

Statistical quantities were computed over a time period $[T_{\text{start}}, T] \subset [0, T]$ were $T_{\text{start}}$ is the time the statistics start being collected and $T$ the final time of the simulation. An ensemble average $\langle (\cdot) \rangle$ is defined as horizontal and time averaged quantities of an arbitrary variable $\phi$

$$\langle \phi \rangle(x_3) := \frac{1}{T - T_{\text{start}}} \int_{T_{\text{start}}}^{T} \left( \frac{1}{8\pi^2} \int_{0}^{4\pi} \int_{0}^{2\pi} \phi(x, t) \, dx_1 \, dx_2 \right) dt.$$  

(5.2)

Furthermore, we define the “bulk” scalar $\phi_b \in \mathbb{R}$ of a quantity $\phi$ as the full average:

$$\phi_b = \frac{1}{2} \int_{-1}^{1} \langle \phi \rangle(x_3) \, dx_3.$$  

(5.3)
5. Numerical results

5.1. Flow cases and non-dimensionalization

Throughout this chapter we consider two different computational setups: three dimensional (3D) full and open channel flows. Channel flows are typical model problems for wall bounded flows with one inhomogeneous direction.

To clarify, we hereby define dimensional quantities with the superscript $^\circ$ and non-dimensional without any extra notation. The full and open channel flow configurations are illustrated in Figure 5.1. Here the dimensional channel half-height $h^\circ$ is introduced which was used to non-dimensionalize the domain $\Omega$. Furthermore, $\langle u_1^\circ \rangle$ is a dimensional streamwise mean velocity.

![Figure 5.1](image)

Figure 5.1: (a) Full channel flow. (b) Open channel flow. Streamwise to wall-normal ($x_1 - x_3$) cross section.

5.1.1. Channel flow

The full 3D channel flow problem can be interpreted as a wall bounded fluid flow between two infinite plates. If the plates are located at $x_3 = \pm 1$ then the full channel domain becomes $\mathbb{R}^2 \times [-1, 1]$. The channel flow configuration is convenient to study for several reasons. First, it yields a statistically steady state result; secondly, the mean streamwise pressure gradient in the channel becomes constant in space and can be applied as an external force to drive the flow. Furthermore, the steady state result of the constant pressure gradient case yields the same Reynolds number as if a constant flow rate is applied. Thus, for the flow to converge to a statistically steady result of a wanted Reynolds number, either a constant pressure gradient may be chosen or the flow rate may be fixed constant. We remark that similar Reynolds numbers from constant pressure gradient and constant flow rate channel flows is only true for an infinite channel, for a periodic channel it is an approximation. However, using a periodic box (as we do) yields statistically accurate ensemble averages $\langle \cdot \rangle$ as long as the domain is large enough to contain the largest turbulent structures of the flow; see e.g. Jimenez et al. (2008).

Non-dimensional velocity quantities $u = \{u_i\}_{i=1}^3$ were obtained by non-dimensionalization using the laminar centerline velocity $\langle u_1^\circ \rangle_{\text{lam}}$ at $x = 0$. An exact laminar solution to a full channel flow problem exists and is a parabola in the
streamwise direction \( x_1 \); it is given by

\[
\langle u_1 \rangle_{|\text{lam}} = 1 - x_3^2.
\] (5.4)

where \( \langle u_1 \rangle_{|\text{lam}} \) is the laminar non-dimensional streamwise solution. Furthermore, the non-dimensional bulk velocity \( u_b \) of the laminar solution of the full channel flow problem becomes:

\[
u_b|_{\text{lam}} := \frac{1}{2} \int_{-1}^{1} \langle u_1 \rangle_{|\text{lam}} \, dx_3 = \frac{2}{3}.
\] (5.5)

Hence, the flow rate \( Q \) for (5.4) simply is \( Q = 2u_b|_{\text{lam}} \). Starting from an intitial condition based on the laminar solution (5.4) and specifying the flow rate as \( Q = 4/3 \) is equal to fix the Reynolds number based on the bulk velocity

\[
\text{Re}_b = \frac{u_b^0 h^0}{\nu_0},
\] (5.6)

where \( \nu_0 \) is a constant kinematic viscosity. Furthermore, the bulk Reynolds number for the simulation is directly linked to the laminar centerline Reynolds number:

\[
\text{Re}_{cl} = \frac{\langle u_1^0 \rangle_{|\text{lam}}(0) h^0}{\nu_0} = \frac{\langle u_1^0 \rangle_{|\text{lam}}(0)}{u_b^0} \text{Re}_b = \frac{3}{2} \text{Re}_b.
\] (5.7)

Moreover, a Reynolds number based on the dimensional friction velocity \( u_f^0 = \nu_0 \rho_0 \partial_3 \langle u_1^0 \rangle_{|\pm1} \) is:

\[
\text{Re}_f = \frac{u_f^0 h^0}{\nu_0} = \sqrt{\text{Re}_{cl} \left| \frac{d \langle u_1^0 \rangle}{dx_3} \right|_{\pm1}},
\] (5.8)

and viscous wall units in the wall-normal direction are defined as:

\[
x_3^+ := \frac{u_f^0 \eta h^0}{\nu_0} = \text{Re}_f \eta, \quad \eta = |x_3| - 1.
\] (5.9)

5.1.2. Open channel flow and atmospheric boundary layers

All high Reynolds number results in this chapter are based on the open channel flow setup. Since the ensemble averaged streamwise velocity (see Equation 5.2) of a channel flow is symmetric along its center-plane it is reasonable to consider only half of the domain. At the center-plane typically free-slip boundary conditions, i.e., homogeneous Neumann for the horizontal velocities and a homogeneous Dirichlet on the vertical velocity, are imposed. These boundary conditions become however an approximation for the instantaneous flow quantities; there are eddies whose height spans through the center-plane. However, comparisons between full and open channel flows show that the open-channel case indeed yields similar horizontal statistics to the closed channel case in most of the domain away from the center-plane; see e.g. Nezu & Rodi (1986). Since we are mainly interested in near wall effects the open channel problem is therefore sufficient. The reason for this is twofold. First, computationally we get a higher resolution close to the boundary using the Chebyshev grid point distribution with the open channel setup and equal resolution. Secondly, the open channel
flow configuration for high Reynolds numbers over a rough surface can be seen as the simplest form of an atmospheric boundary layer without Coriolis force (as e.g., regions close to the equator). Typical atmospheric boundary layer simulations utilize the same type of boundary conditions: periodic on the sides, free-slip on top, and a wall model on bottom boundary; see e.g. Moeng (1984) or Bou-Zeid et al. (2005). We should remark here that for boundary layers there is a spatial increase in boundary layer height, whereas in an open channel flow the height is fixed. However, due to the very high Reynolds numbers the height increase can be negligible. The height increase can be estimated in terms of Reynolds number \( \text{Re}_x := \frac{U_\infty x_1}{\nu} \) \((\text{U}_\infty \text{ free-stream velocity})\) as \( \text{Re}_x^{-0.8} \) (see e.g. Schlichting 1968), which becomes very close to zero for a Reynolds number in the ABL range (\( \text{Re}_x \approx 10^6 \) and up).

The non-dimensionalization for an open channel flow is similar to the full channel. We consider the non-dimensional domain \( \Omega \) that were non-dimensionalized with the channel half height \( h^o \) (see Figure 5.1b). Since we have the Chebyshev points with range \([-1,1]\) it is however convenient to define a coordinate transformation \( f : [0,h] \mapsto [-1,1] \) given by \( f(x) = -1 + 2x/h \). Thus, first a shift then a division by \( h/2 \). The laminar solution now is

\[
(u_1)_{\text{lam}} = \frac{(x_3 + 1)^2}{4}.
\]

And the non-dimensional bulk velocity here becomes half that of the open channel, i.e., \( u_b = 1/3 \). The Reynolds numbers of the open channel case simply becomes half that of the full channel for the same \( h^o \) and \( \nu_0 \).

5.2. General effects of slip boundary conditions in low Reynolds number turbulent channel flows

In a first set of simulations we consider direct numerical simulations of a low Reynolds number turbulent full channel flow. Here the domain \( \Omega \) is discretized over \( 128^2 \times 129 \) grid points (similar to e.g. Kim et al. 1987). This resolution is sufficient for a DNS to consider the main effects. The partial slip and no penetration boundary conditions (see §3.3.1) are applied on the upper and lower wall boundaries:

\[
u_3 = 0; \quad \beta_j u_j + \frac{\partial u_j}{\partial x_3} = 0, \quad j = 1, 2, \quad x_3 \in \{-1,1\}.
\]

A constant flow rate was chosen as \( Q = 4/3 \) together with a bulk Reynolds number of \( \text{Re}_b = 2800 \) which corresponds to \( \text{Re}_\tau \approx 180 \) (Dean 1978). An initial simulation with no-slip boundary conditions was run with an initial condition chosen as the exact laminar solution \( u_1 = 1 - x_3^2 \) with superimposed noise to trigger turbulence. The result of this initial simulation was then used as an initial condition for the rest of the runs and for comparison. Simulations with the following combinations of friction coefficients were considered: \((\beta_1, \beta_2) \in \{(10, \infty), (10, 10), (25, \infty), (25, 25), (100, \infty), (100, 100)\}\) where \( \infty \) means \( u_3 = 0 \). Several more combinations were also studied, but no extra additional information was obtained.
5.2. General effects of slip boundary conditions

We should stress here that with this example we aim to consider the effect of the slip boundary conditions and their potential in wall modeling for high Reynolds number simulations. Channel flow studies of \( \text{Re}_\tau = 180 \) (as well as \( \text{Re}_\tau = 360 \)) have already been conducted with slip boundary conditions, then with main interest in drag reducing and drag increasing mechanisms. Well cited papers are the very short one by Min & Kim (2004) and the more extensive study by Busse & Sandham (2012).

From the definition of the Robin conditions (5.11) it is given that a slip velocity in the streamwise direction influences the near-wall wall-normal derivative and thus the near-wall shear stress. A small streamwise friction coefficient leads to a small derivative and vice versa. This is also verified by plotting the streamwise mean profiles; see Figure 5.2. In the plots, the scaling \( u_{\tau,0} \) is defined as the friction velocity \( u_\tau \) of the no-slip case. Furthermore, In Figure 5.3 the mean profiles are plotted in log-scale for streamwise as well as both streamwise and spanwise slip. We plot both \( \langle u_1 \rangle / u_{\tau,0} \) (as in Figure 5.2) and also \( (\langle u_1 \rangle - \langle u_1 \rangle|_{\text{wall}})/u_{\tau,0} \). Here the former can be used to consider the effect of the slip on the outer layer and the latter for the effect of the slip in the viscous wall region. It is evident that the presence of slip to a higher extent seems to influence the viscous wall region. With an additional spanwise slip condition we can further note that we indeed get an increase in the overall slip velocity in the streamwise direction. In Figure 5.3b we can note that the effect of the spanwise slip also seems to start have an impact inside the buffer/lower logarithmic regions of the channel.
Figure 5.3: Streamwise mean velocity profiles. Streamwise slip only (solid) versus streamwise and spanwise slip (dotted). Bold line is the no-slip case.
5.2. General effects of slip boundary conditions

An interesting quantity that regards the mean profile and provides information about the suitability of the slip boundary conditions as potential wall models is the log-indicator function \( \Phi(x^+ + 3) := x^+ \frac{dU^+}{dx^+} \), where \( U^+ := \langle u_1 \rangle / u_T \). It indicates to what extent the mean profiles follow a logarithmic behavior. For a logarithmic behavior \( \Phi(x^+_3) \) becomes equal to \( 1/\kappa \approx 2.6 \). In Figure 5.4 we plot \( \Phi(x^+_3) \); we still use \( u_{r,0} \) as the scaling. It is clear that the slip boundary conditions increase the logarithmic behavior of the solution with an increased slip velocity. As we can see in Figure 5.3b, the addition of a spanwise slip make the normal derivative of \( \Phi \) smaller in the buffer region which indicates a more extensive logarithmic behavior. This result gives a positive indication for using slip boundary conditions as wall models for LES where the viscous sublayer cannot be resolved. Remark though that a logarithmic behavior all the way down to the surface is not possible here as the logarithmic function is undefined at the origin (\( \log(x) \to -\infty \) as \( x \to 0 \)).

In Figure 5.5 we furthermore consider the turbulence intensity statistics. Not surprisingly, a streamwise slip makes the turbulence production due to shear lower; the peak in the streamwise root-mean-square (RMS) velocity \( \sqrt{\vec{u}_1 \cdot \vec{u}_1} / u_{r,0} \) (Figure 5.5a) decreases with an increased slip. Even more interestingly is that a
Figure 5.5: Streamwise (a) and spanwise (b) rms velocities. Streamwise slip only (solid) versus streamwise and spanwise slip (dotted). Bold line is the no-slip case.
spanwise slip indeed increases the streamwise turbulence intensity. Moreover, considering the spanwise turbulence intensities (Figure 5.5b) we see that indeed an increase in spanwise slip increases the spanwise turbulence intensity which is the opposite to the streamwise case. A remark for these results is the scaling. The differences between the different cases do depend on the non-dimensionalization by $u_{\tau,0}$. However, from the mean profile results we we could see that the scaling $u_{\tau,0}$ makes the different results collapse in a point around $x_3^+ \approx 60-80$. That for a $Re_\tau \approx 180$ channel flow is (if such exists) in the lower part of logarithmic region.

To get more insight into potential effects of the slip boundary conditions on the simulated turbulence we further consider instantaneous horizontal planes for the streamwise velocities; see Figure 5.6. These were collected at the final time of the simulation. We compare the slip velocities for different $\beta_j$ and compare these with the streamwise velocity fields taken from the no slip simulation at four different heights $x_3 \in \{0.048, 0.0585, 0.1068, 0.5724\}$ (or in wall units $x_3^+ \in \{0.86, 10.53, 19.22, 103.03\}$). We can see that, in the $\beta_j = 10$ cases where the slip velocity is large and turbulence intensity rather low the flow structures are elongated but wide and smooth with large maximum velocity. Decreasing the slip velocity and therefore increasing the shear, leads as expected to smaller and smaller maximum velocities but also more significant streaky structures. Compared to the streamwise slip only, an addition of a spanwise slip shows up in the instantaneous turbulence as more spanwise variation and larger maximum slip velocities. Compared to the no-slip fields we can see that the turbulent structures at the wall for the slip boundary condition cases are larger than the streaks close to the wall for the no-slip case. As is most clearly seen for the $\beta_1 = \beta_2 = 25$ field, the slip velocity field has structures that are comparable (roughly) in length and width to the no-slip result at $x = 0.1068$ (or $x_3^+ = 19.22$) which were the turbulence intensity is largest (see Figure 5.5). Thus the structures at the slip boundary has potentially the right shape to bypass the viscous wall region. However the magnitude of the turbulence intensity is still much lower for the slip velocity than the DNS result.

5.2.1. Summary

Slip boundary conditions were tested in a low Reynolds number turbulent channel flow ($Re_\tau = 180$). The streamwise mean flow statistics are in line with literature such as Min & Kim (2004) and Busse & Sandham (2012). A streamwise slip gives a reduced near-wall stress and a decrease in the turbulence intensity. An addition of spanwise slip on the other hand increases the turbulence intensity in both the streamwise and spanwise directions together with a slight increase in the streamwise mean velocity. The slip boundary conditions controls the shear at the boundary; an increased slip velocity is equivalent to a lower shear and the other way around. We plotted the log-indicator function and could see that with slip boundary conditions the mean profiles becomes closer to logarithmic through the viscous wall region. By plotting instantaneous fields
5. Numerical results

Figure 5.6: Instantaneous streamwise velocity planes. The first three rows correspond to the \( x_3 = 0 \) boundary plane for simulations with different slip lengths (slip velocities). And the lower two rows correspond to the no-slip simulation at four different heights \( x_3 \in \{0.0048, 0.0585, 0.1068, 0.5724\} \) (or in wall units \( x_3^+ \in \{0.86, 10.53, 19.22, 103.03\} \)).
of the slip velocity at the boundary plane we could see turbulent structures that are smoother than typical inner layer streaks with horizontal lengths and widths that approximately match the ones in the upper buffer layer/logarithmic regions. We can conclude that the influence from the spanwise slip condition becomes important from a wall modeling perspective as it increases the logarithmic behavior in the viscous wall region and furthermore increases the streamwise turbulence intensity (which decreases for a streamwise slip only). Thus, as a wall model slip boundary conditions would be used for both streamwise and spanwise velocity quantities.

5.3. LES of high Reynolds number open channel flows

We now move to a more relevant flow case in terms of atmospheric flows. In this section we consider the open channel configuration for a high Reynolds number LES. We use a simple Smagorinsky eddy-viscosity model to close the SGS stress tensor and study the performance of the slip boundary conditions together with the the wall stress matching function of Mason et al. presented in §3.4.

5.3.1. Computational setup

Through this section the over-bar \( \bar{\cdot} \) defines a LES filtered quantity and the hat \( \hat{\cdot}(k, x_3, t) \) a horizontally \((x_1 - x_2)\) Fourier transform where \( k = (k_1, k_2)^\top \) are horizontal wavenumbers (see §4.1.3). The domain of study is the non-dimensional \( \Omega \) given in Equation (3.4).

For the sake of simplicity in the explanation below, we map the coordinates in the vertical direction as follows: \([-1, 1] \mapsto [0, 1]\). In the code we solve over \([-1, 1]\) though, and the non-dimensionalization need to take that factor two in mind. For instance, the height of the domain is here \( h^o \). Non-dimensionalization of e.g., the roughness height \( h^r \) will then be \( h_r = h^r/h^o \). However, in the code we need to use \( 2h_r \).

We consider the boundary conditions that were presented in §3.3.3 which separates friction coefficients for the partial slip conditions between the zero and non-zero wavenumbers. We here present the boundary conditions in Fourier transformed quantities like they are imposed in the code. On the upper boundary \( x_3 = 1 \) we impose a free-slip boundary condition

\[
\frac{\partial}{\partial x_3} \hat{u}_1(k, 1, t) = \frac{\partial}{\partial x_3} \hat{u}_2(k, 1, t) = \hat{u}_3(k, 1, t) = 0, \quad \forall (k, t). \quad (5.12)
\]

And on the lower boundary \( (x_3 = 0) \) we impose the proposed partial slip and no penetration boundary conditions (see §3.3.3):

\[
\begin{align*}
\beta_j \hat{u}_j(0, 0, t) + \frac{\partial}{\partial x_3} \hat{u}_j(0, 0, t) &= 0, \quad j = 1, 2, \\
\gamma_j \hat{u}_j(k, 0, t) + \frac{\partial}{\partial x_3} \hat{u}_j(k, 0, t) &= 0, \quad j = 1, 2, \quad k \neq 0, \\
\hat{u}_3(0, 0, t) &= 0, \quad \forall k
\end{align*}
\quad (5.13)
\]
Here \( \{\beta_j\}_{j=1,2} \) are friction coefficients corresponding to the zero wavenumber, and \( \{\gamma_j\}_{j=1,2} \) friction coefficients corresponding to the non-zero wavenumbers. The initial condition is here chosen as a logarithmic profile in the streamwise direction with a a fixed flow rate \( Q = 4/3 \) (zero for the spanwise and vertical velocities)

\[
\hat{u}(k, x_3, 0) = \begin{pmatrix}
\frac{Q \log \left( (\delta h + x_3)/h_r \right)}{\log \left( ((\delta h + 1)/h_r) + \delta h \log \left( (\delta h + 1)/\delta h \right) - 1 \right)} \\
0 \\
0
\end{pmatrix}, \tag{5.14}
\]

which is superposed with random noise to trigger turbulence. Here, \( \delta h \) is the non-dimensional height of the roughness region below the boundary (or simply said, the artificial boundary height; see §3.3) and \( h_r \) a non-dimensional empirical roughness height. For the dimensional quantities used in the non-dimensionalization we assume according to a typical atmospheric boundary layer (see e.g., Moeng (1984) or Garratt (1992)) a constant velocity at the upper boundary of \( U^\circ_h = 10 \) [m/s] (similar to a geostrophic wind), a height of the domain of \( h^\circ = 1000 \) [m] and the roughness height \( h^c_r = 0.1 \) [m]. Thus, a Reynolds number for the flow can be defined as

\[
\text{Re}_h = \frac{U^\circ_h h^\circ}{\nu_0} \approx \frac{10 \times 1000}{1.25 \times 10^{-5}} = \mathcal{O}(10^9), \tag{5.15}
\]

This Reynolds number gives a viscous term in the Navier–Stokes equations of magnitude \( \mathcal{O}(10^{-9}) \) which becomes negligible small. To overcome stability and accuracy problems we introduce according an artificial viscosity (here chosen as \( \tilde{\nu} = 0.001 \); see §4.4) and model all stress through the eddy-viscosity model.

Furthermore, the non-dimensional roughness height becomes

\[ h_r = h^c_r/h^\circ = 0.0001, \]

and the non-dimensional artificial boundary height \( \delta h \) is computed from the modeling expression of the streamwise friction coefficient

\[ \beta_1 = -1/(\delta h \log(\delta h/h_r)), \]

In table 5.1 we present \( \delta h \) and \( \delta h^c \) for different \( \beta_1 \).

<table>
<thead>
<tr>
<th>( \beta_1 )</th>
<th>( 10 )</th>
<th>( 20 )</th>
<th>( 50 )</th>
<th>( 100 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \delta h )</td>
<td>0.0107</td>
<td>0.00609</td>
<td>0.00296</td>
<td>0.00175</td>
</tr>
<tr>
<td>( \delta h^c ) [m]</td>
<td>10.7</td>
<td>6.09</td>
<td>2.96</td>
<td>1.75</td>
</tr>
</tbody>
</table>

The main interest of this study is to consider the effect of slip boundary conditions in a model problem for an atmospheric boundary layer, i.e., a high Reynolds number wall bounded flow where the viscous wall region is completely
under resolved. Like in the previous low Reynolds number DNS study we do several simulations for different combinations of the boundary condition parameters. We consider different $\beta_j$ but now also different $\gamma_j$.

The SGS model is here chosen as the standard Smagorinsky model with the Smagorinsky coefficient chosen as $C_s = 0.1$. Simulations were conducted both with and without the Mason et al. stress matching function.

The turbulence statistics (ensemble averages; see (5.2)) are presented non-dimensionalized with either the bulk velocity $\bar{u}_b$ (see (5.3)) or a friction velocity $u_\tau$. The bulk velocity is directly given since we fix the mass flow rate. In the simulations we solve for $\bar{u} = \bar{u}^\circ / U_h^\circ$. The bulk velocity is given by $\bar{u}_b = \bar{u}_b^\circ / U_h^\circ = 2/3$. Thus, $\langle \bar{u}^\circ \rangle / \bar{u}_b^\circ = \langle \bar{u} \rangle / \bar{u}_b = (3/2) \langle \bar{u} \rangle$. However, since we use wall boundary conditions with the aim of relaxing the no-slip condition it is not reasonable to compute $u_\tau$ from the wall derivative. Instead we compute $u_\tau := u_\tau^\circ / U_h^\circ$ by assuming that the logarithmic law holds at the artificial boundary (at $\delta h$) and use a von Kármán constant $\kappa = 0.4$ to estimate $u_\tau$:

$$u_\tau := \frac{\kappa \langle \bar{u}_1 \rangle |_{x_3=0}}{\log(\delta h/h_\tau)}.$$  \hspace{1cm} (5.16)

We need to stress here that $u_\tau$ is used only in a post-processing step. We do not use $u_\tau$ for the modeling as e.g., the Moeng wall-stress model does. The way we define $u_\tau$ is only important when we study and compare results. Computing it at the boundary and assuming that the logarithmic law holds there is true locally according to the definition of the slip conditions and give us an indicator on how well the flow react to the boundary conditions. Non-dimensionalizing with the bulk velocity on the other hand gives a better global view. How we scale is really a matter of what we want to study.

In nothing else is mentioned the resolution of the simulations in this section is chosen as $64^2 \times 65$ which is neither very coarse or dense for a wall modeled LES and similar to what other use for the same type of simulations (see e.g. Bou-Zeid et al. 2005). This resolution provided us with converged statistics in some hours on a 28 core machine using OpenMP parallelization.

In all simulations the streamwise and spanwise friction coefficients were chosen equal to each other, i.e., $\beta := \beta_1 = \beta_2$ and $\gamma := \gamma_1 = \gamma_2$. This was chosen with the results from the previous section in mind. Also, in terms of numerical stability for the large eddy simulations we have experienced the Robin conditions gives overall more stable results than Dirichlet. Thus, we never use a Dirichlet condition for the spanwise velocity.

### 5.3.2. Importance of wall stress matching

In §3.4 we reviewed some wall functions that are commonly used in LES. In context of wall modeled LES of atmospheric boundary layers the mixing length matching function first presented by Mason et al. was stated as

$$l_s(x_3) = \left[ l_0^{-\alpha} + l_m (x_3 + \delta h)^{-\alpha} \right]^{-1/\alpha}, \quad \alpha \in \mathbb{R}^+,$$  \hspace{1cm} (5.17)
where \( l_0 = C_S \delta_S \) is a fixed Smagorinsky length scale in the outer layer with \( \delta_S = (\delta_1 \delta_2 \max_{x_3} \delta_3)^{1/3} \), and \( l_{\text{ml}}(x) := \kappa x \) a mixing length function. The parameter \( \alpha \) defines the strength of the matching and is usually chosen between one and four, where the most common choice is \( \alpha = 2 \).

In this subsection we test the performance of this mixing length matching function (5.17) together with slip boundary conditions. We consider results computed with the Smagorinsky model with and without matching function applied. In these first simulations the friction coefficients were here chosen similar for all wavenumbers, i.e. \( \beta = \gamma \). The reason we chose the friction coefficients equal here is first of all to start with the simplest case, but also to be consistent with a boundary condition implemented in physical space. These results should be comparable to what is possible to obtain also with other numerical codes. All statistics are non-dimensionalized width the bulk velocity \( \bar{u}_b = 2/3 \) and compared to the largest published DNS channel flow result available, i.e., the \( \text{Re}_\tau \approx 5200 \) study by Lee & Moser (2015). Even though this DNS result is the highest available the Reynolds number is still low compared to an atmospheric flow. However, since the Smagorinsky model is unchanged for different Reynolds numbers we claim that in a coarse grid LES we cannot expect much of a difference in the result if \( \text{Re}^{-1} \) is \( 10^{-9} \) or approximately zero. In the total dissipation \( \text{Re}^{-1} + \nu_t \) the eddy-viscosity becomes of several orders of magnitude larger than \( \text{Re}^{-1} \) especially in the near wall region where the vertical gradient is high.

In the rest of this chapter we use the following scaling of the vertical coordinates. The total height is defined as: \( \bar{h}^\circ := h^\circ + \delta h^\circ \). Furthermore, we let \( \delta \bar{h} := \delta h/(h + \delta h) \). Corresponding vertical non-dimensional coordinates becomes: \( \bar{x}_3 := (x_3^\circ + \delta h^\circ)/h^\circ \in [\delta \bar{h}, 1] \). This scaling is employed for all plots where wall boundary conditions are located at a non-zero height.

The streamwise mean velocity profiles for \( \beta \in \{10, 50, 100\} \) are shown in Figure 5.7 together with the Lee & Moser (2015) result. Noticeable variations can be seen in results computed with a the Smagorinsky model without matching function; see Figures 5.7a and 5.7c. For the largest slip case \( \beta = 10 \), a too large slip velocity is seen at the computational boundary compared to the DNS result. The stress becomes also clearly too low in the outer layer. For \( \beta = 50 \) and 100 the profiles in the outer layer are more reasonable. However, with smaller slip a significant spurious viscous effects is clearly seen in these results. This spurious region becomes less pronounced with an increased slip mainly since the height of it stays approximately the same. Clearly there is no universal choice of friction coefficient in terms of accuracy for the Smagorinsky-only case.

If a matching function is applied the results improves drastically in terms of \( \beta \) dependency; see Figures 5.7b and 5.7d. The streamwise mean profiles for \( \beta = 50 \) and 100 collapses under each other and only a small deviation can be seen between these and the large slip case \( \beta = 10 \). Compared to the Smagorinsky-only case the spurious inner region for the \( \beta = 50 \) and 100 results
Figure 5.7: Streamwise mean velocity profiles. \{(a),(c)\} original Smagorinsky model; \{(b),(d)\} Smagorinsky model with Mason et al. matching function (Equation 5.17). The slip boundary conditions were here chosen equally for all wavenumbers, \(i.e., \beta = \gamma\). LM2015 is the \(\text{Re}_x \approx 5200\) channel flow result by Lee & Moser (2015).
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Figure 5.8: As in Figure 5.7 but for streamwise turbulence intensity profiles.
are now much less pronounced; close to the computational boundary there is now also a more evident logarithmic behavior.

In Figure 5.8 we further plot the streamwise turbulence intensities, also here non-dimensionalized with the bulk velocity for comparison against the Lee & Moser (2015) DNS result. Similar to the mean profiles there is here a big spread in the Smagorinsky-only results. The $\beta = 10$ case has a turbulence intensity that is almost an order of magnitude lower than both the $\beta = 50$ and $\beta = 100$ results, which on the other hand have too high turbulence intensities compared to the DNS result. The optimal choice is probably for a $\beta$ somewhere in between 10 and 50. Considering the results computed with the matching function the turbulent intensity curves are much closer to each other and all of approximately similar magnitudes as the DNS case. A larger slip (or smaller shear) gives however a decrease in turbulence intensity also here. However the $\beta = 50$ and 100 results are closer to each other than for the Smagorinsky-only cases. These results are also in line with the DNS results in the previous section. We should however be careful to draw too strict conclusions since the spread depend on the choice of scaling.

In all the turbulence intensity curves presented in Figure 5.8 there is a clear peak in the near-wall region. Such a peak is also seen in the Lee & Moser (2015) DNS result but then appears closer to the wall. It is well known that this peak corresponds to the maxima in turbulence production and is located inside the viscous wall region. In a wall modeled LES such peak therefore becomes a spurious viscous layer effect and is indeed a well known problem (see e.g. Sagaut 2006). Computationally the peak is partly a direct result of the boundary conditions. It is clear that since we enforce a positive gradient for all wavenumbers such a peak must exist. This was also discussed in §3.3.3, and an attempt to eliminate this peak will soon be provided (see §5.3.3).

To understand the poor performance of the Smagorinsky model without matching function we can do some quick calculations. We compare the mean eddy-viscosity produced by the Smagorinsky model at the wall with that of the imposed mixing-length for the matching function (which furthermore equals to the logarithmic law for the averaged velocity). The ensemble averaged eddy-viscosity at $\delta h$ is

$$\langle \nu_t \rangle = (C_S \delta S)^2 \langle |\nabla^s \bar{u}| \rangle \approx (C_S \delta S)^2 \frac{d \langle \bar{u}_1 \rangle}{dx_3}. \quad (5.18)$$

Thus, the only way the Smagorinsky model can match the stress of the logarithmic law is if $C_S \delta S \approx \kappa \delta h$. Different values of these quantities for the simulations corresponding to the results in Figures 5.7–5.8 are presented in Tables 5.2 and 5.3. Comparing the mixing lengths in Table 5.2 with the Smagorinsky lengths in Table 5.3 for the artificial boundary $\delta h$ we see that in the actual situation $64^2 \times 65$ and $C_S = 0.1$ only the $\beta_1 = 50$ case gives a reasonable approximation. This is also consistent with our observations in Figures 5.7 and 5.8. For a $\beta_1 = 10$, the standard Smagorinsky model yields a length scale that
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Table 5.2: Mixing lengths for different friction coefficients. This is what the code see, it is without the mapping \([-1,1] \mapsto [0,1]\). We have \(\delta h^\dagger := 2\delta h\).

<table>
<thead>
<tr>
<th>(\beta_1)</th>
<th>10</th>
<th>20</th>
<th>50</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\kappa \delta h^\dagger)</td>
<td>0.00856</td>
<td>0.00489</td>
<td>0.00236</td>
<td>0.00140</td>
</tr>
</tbody>
</table>

Table 5.3: Filter widths for the Smagorinsky model \(\delta_S^\dagger = (\delta_1 \delta_2 \delta_3^\dagger)^{1/3}\) at the boundary for different grid resolutions and Smagorinsky coefficients \(C_S\). Similar as in Table 5.2, this is without the mapping \([-1,1] \mapsto [0,1]\); thus \(\delta_3^\dagger := 2\delta_3\).

<table>
<thead>
<tr>
<th>(N_1 \times N_2 \times N_3)</th>
<th>(32^2 \times 33)</th>
<th>(64^2 \times 65)</th>
<th>(128^2 \times 129)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\delta_S^\dagger\mid_{x_3=0})</td>
<td>0.07187</td>
<td>0.0285</td>
<td>0.01132</td>
</tr>
<tr>
<td>(0.1 \delta_S^\dagger\mid_{x_3=0})</td>
<td>0.00719</td>
<td>0.00285</td>
<td>0.00113</td>
</tr>
<tr>
<td>(0.17 \delta_S^\dagger\mid_{x_3=0})</td>
<td>0.01222</td>
<td>0.00485</td>
<td>0.00192</td>
</tr>
</tbody>
</table>

is approximately three times too large (0.00856 vs 0.00285) which leads to a too high stress compared to the logarithmic law. The \(\beta_1 = 100\) case on the other hand yields a length scale that is approximately half that (0.00140 vs 0.00285) of the mixing length model and thus a too low stress. This shows up in the mean profiles and is even more clear in the turbulence intensities. Moreover, in the tables above also the \(C_S = 0.17\) case was added for comparison. Clearly, changing \(C_S\) gives a higher overall length-scale for the Smagorinsky model and another result since the Smagorinsky length scale depends on both \(\delta_S\) and \(C_S\); some further testing on that will further be presented in §5.3.4.

5.3.3. Eliminating the “spurions peak”

Recall, in the turbulence intensity plots of Figure 5.8 we could notice a “spurious peak” that shows up as an artificial viscous layer effect. In this subsection we study the effects of imposing different friction coefficients on the zero and non-zero wavenumber boundary conditions (\(\beta_j\) and \(\gamma_j\) in (5.13)) separately to control the turbulence intensity statistics in the near-wall region. The simulations performed here are similar to them in the previous subsection except for the parameter changes in the boundary conditions and that we now use a matching function for all cases.

To see the variations in the results for different non-zero wavenumber friction coefficients \(\gamma\) we fix the zero wavenumber friction coefficient to \(\beta = \beta_1 = \beta_2 = 50\). For the the matching function (5.17) the \(\alpha\) parameter is initially chosen as \(\alpha = 2\).

Consider in Figure 5.9 the streamwise turbulence intensity statistics. It is evident that by changing the boundary conditions for the non-zero wavenumbers
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Figure 5.9: Streamwise turbulence intensity (solid lines). The zero wavenumber friction coefficient is set to $\beta_1 = \beta_2 = 50$ and the non-zero wavenumber friction coefficients $\gamma_1 = \gamma_2$ are changed in a step-wise manner. The dotted line is the $Re_\tau \approx 5200$ channel flow result by Lee & Moser (2015).

we can control the vertical derivative of the streamwise turbulence intensity at the boundary. This is also in line with our calculations in §3.3.3; the derivative of the streamwise turbulence intensity is directly linked to the friction coefficients $\gamma_1$ and $\gamma_2$. Fortunately, the slip boundary conditions seem to work as expected. We can impose conditions that gives us control over the derivatives and velocities at the computational boundary also for fluctuations. Indeed, for a negative $\gamma = \gamma_1 = \gamma_2$ the spurious peak in the streamwise turbulence intensity becomes completely eliminated.

For further comparison we non-dimensionalize the results with the locally computed friction velocities $u_\tau$ (Equation (5.16)) and compare the results to the logarithmic profile according to the attached eddy hypothesis (AEH); see Figure 5.10. The AEH inverse logarithmic expression for the turbulent intensity reads

$$\frac{\langle u_1'^2 \rangle}{u_\tau^2} = B_1 - A_1 \log(\bar{x}_3)$$

in which the parameters were taken as $A_1 = 1.33 \pm 0.17$ and $B_1 = 2.14 \pm 0.40$ corresponding to data from SLTEST atmospheric boundary layer measurements; see Hutchins et al. (2012) and Marusic et al. (2013). In Figure 5.10 the variance in $\langle u_1'^2 \rangle/u_\tau^2$ to the uncertainty in $A_1$ and $B_1$ was added as a gray area. Compared to the logarithmic curve we get for the $\gamma = -5$ case a turbulence intensity that is overall a bit high. There may be several reasons for this. For sure
Figure 5.10: Streamwise turbulence intensity (solid lines) plotted in log-scale and scaled with the estimated friction velocity $u_τ$ (Equation (5.16)). The dark gray line and the gray filled region correspond to the SLTEST attached eddy expression from Marusic et al. (2013). Dotted line is the DNS channel flow by $\text{Re}_τ \approx 5200$ channel flow result by Lee & Moser (2015). The dashed line is the $γ = −5$ result but scaled with a friction velocity assuming $κ = 0.438$ instead of 0.4 according to the maximum deviation of the SLTEST measurements.

There is the SGS modeling dependency but there is also an ambiguity in the non-dimensionalization which plays in. Choosing the von Kármán constant larger gives a larger estimation of the friction velocity by Equation (5.16) and a smaller turbulence intensity. In SLTEST the von Kármán constant was measured as $0.410 \pm 0.028$. A small improvement in the results can be obtained by picking the upper limit $0.438$ instead of the general von Kármán constant value 0.4; see the dashed line in Figure 5.10.

The effects of the changes in the $γ$ parameter on the mean profile is further examined in Figure 5.11 where the logarithmic profiles and also the relative error of the derivative against the logarithmic law $U_{\text{log}} := u_τ/(κ\bar{x}_3)$ are plotted. The relative error was computed against the logarithmic law obtained by the $u_τ/κ$ estimated at the artificial boundary $δ\bar{h}$ from the following expression

$$
\left( \frac{d\langle \bar{u}_1 \rangle}{d\bar{x}_3} - \frac{dU_\text{log}}{d\bar{x}_3} \right) / \frac{dU_\text{log}}{d\bar{x}_3} = \frac{d\langle \bar{u}_1 \rangle}{d\bar{x}_3} / \frac{dU_\text{log}}{d\bar{x}_3} - 1
$$

$$
= \left( \frac{d\langle \bar{u}_1 \rangle}{d\bar{x}_3} \right) / \left( \frac{d\langle \bar{u}_1 \rangle}{d\bar{x}_3} \right)_{\delta\bar{h}} - 1
$$

We can note in Figure 5.11 that when $γ$ is decreased the logarithmic fit becomes slightly improved. There is still a spurious viscous layer effect, but it is reduced.
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\[ \gamma \in \{50, 25, 10, 0, -5\} \]

\[ \frac{\langle u_1 \rangle}{\bar{u}_b} \]

\[ 10^{-2} \quad 10^{-1} \quad 10^0 \]

\[ x_3 \]

\[ \frac{d\langle u_1 \rangle}{dx_3} - \frac{d\langle \log \rangle}{dx_3} \]

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

\[ \gamma \in \{50, 25, 10, 0, -5\} \]

Figure 5.11: Effect of changing the \( \gamma \) parameter on the streamwise mean profile. (a) mean profiles in log scale, (b) relative error of the vertical derivative of the mean profiles in (a).

5.3.4. Smagorinsky length scale dependency

At this point we have seen the potential in using slip boundary conditions for high Reynolds number wall modeled LES. The focus has been in testing these and we have not spent much effort in the SGS modeling part which we chose in the simplest possible way as a Smagorinsky model with \( C_S = 0.1 \). However, the wall boundary conditions can only provide us with a solution for the specific equations they are imposed for. In fact, the impact of the Smagorinsky model becomes significant in our high Reynolds number simulations. As explained in §2.2.2, the Smagorinsky model provides us with a set of approximate grid filtered equations. Thus, changing the Smagorinsky model means that we solve for another type of “Smagorinsky fluid”. If the Smagorinsky fluid flow approximates a real fluid flow problem depends on how the parameters of the Smagorinsky model are chosen. Different testing and/or dynamic procedures (Germano et al. 1991) can be used to approximate parameters for the Smagorinsky model. However, for this high Reynolds number and for boundary layer flows in general there are no perfect approximations available. Our intention in this thesis is not to spend much time in ad-hoc tuning of parameters or averaging principles for a dynamic Smagorinsky model. What is a right setup for one specific situation may not be so in another. However, what we are interesting in is the impact of the modeling. We want to find a more general setup that is robust enough to be used for most cases and where the effects hopefully can be understood mathematically. A stress-matching function is one step in the right direction in this sense. It increases the robustness of the near wall solution and makes the modeling more universal.
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Even though weak type of boundary conditions (Robin conditions) and a matching function are employed we could still experience some viscous layer effects in the streamwise mean profiles. This we could see in Figure 5.11. By observation, this inner layer effect can be explained as a too low stress level at a small distance above the artificial wall. The magnitude of the stress in our Smagorinsky LES simulations is directly linked to the Smagorinsky length scale \( l_S \). Thus, it is reasonable to do some testing to see if the spurious effect can be reduced even further by modifying \( l_S \).

Recall here that the Smagorinsky length scale depends on how the Smagorinsky coefficient \( C_S \) is modeled but also how the filter width \( \delta_S \) is defined. It does not matter if one of these is chosen in a very detailed way if the other is picked roughly. If a matching function is employed it is on the other hand the total effect of \( l_S \) that is modeled. Instead of letting \( C_S \) and the (possible non-uniform) grid-spacing determine the wall normal variation in \( l_S \) as a wall boundary is approached we instead fix \( l_S \) at the boundary and let it smoothly vary to a fixed value further out. The transition of \( l_S \) by the matching function is unfortunately not physical but it can be controlled by the matching parameter \( \alpha \). Initially we did choose \( \alpha = 2 \) which is also the value proposed in the original papers by Mason et al. But the \( \alpha = 2 \) choice lacks justification and further depends on scaling.

In Figure 5.12 we plot the streamwise mean profile and relative error again. Now for three different matching parameters: \( \alpha \in \{1, 1.5, 2\} \). We can see...
that a smaller $\alpha$ (which corresponds to a less steep matching) gives a better logarithmic fit. The spurious viscous layer effect is still there but reduced. As mentioned in §3.4.2, a small $\alpha$ does not give a perfect match to the mixing length. This phenomenon starts to show for $\alpha = 1$; see Figure 5.13. This explains the small deviation from the logarithmic behavior in the first few points for that case. The error is however quite small compared the deviations further up in the domain, and would be corrected by a small shift in the matching function formulation; however, for simplicity we here simply used the uncorrected version. In Figure 5.12 the result of an increase in $C_S$ was also plotted. We here used the Lilly (1967) value $C_S = 0.17$ for comparison. It is clear that as $C_S$ increases the height of the spurious viscous layer increases as well. This effect is expected since we let the eddy-viscosity account for all viscous contributions. The physical viscous sublayer becomes thinner with an increased Reynolds number; it is therefore reasonable that reducing the magnitude of the eddy-viscosity should lead to a similar effect for the LES. And since the magnitude of the eddy-viscosity can be directly linked to the Smagorinsky length scale it becomes directly influence by $C_S$.

In Figure 5.14 we furthermore plot the streamwise turbulence intensity for the $\alpha$ and $C_S$ changes. With a decrease in $\alpha$ the streamwise turbulence intensity becomes overall smaller and in magnitude closer to what the attached eddy hypothesis suggests (assuming that the scaling is appropriate). An increased $C_S$ gives a larger turbulence intensity in regions of the boundary layer that is neither close to the wall or close to the upper boundary. This can be explained by the fact that close to the wall boundary the mixing length formulation through the matching function is universal, there is only a little impact of a changed $C_S$ there, and close to the upper wall the vertical gradient is small.
Figure 5.14: As Figure 5.11 but for the streamwise turbulence intensity. Solid lines correspond to $\alpha \in \{1, 1.5, 2\}$ and $C_S = 0.10$. The dashed lines correspond to $\alpha \in \{1, 2\}$ and $C_S = 0.17$. The dotted line represents the Lee & Moser (2015) Re$_\tau \approx 5200$ DNS channel flow result and the dark-gray line and gray region correspond to the attached eddy hypothesis inverse log-law; similar to Figure 5.10.

5.3.5. Instantaneous planes

In Figure 5.15 horizontal planes of the streamwise velocity defect $(\bar{u}_1 - \langle \bar{u}_1 \rangle) / \bar{u}_b$ are plotted for three heights $\hat{x}_3 \in \{\delta \hat{h}, 0.095, 0.40\}$ for simulations with $\beta = \gamma = 50$ and $\beta = 50$ and $\gamma = -5$ as slip boundary condition parameters at the final time of the simulations. The height $\hat{x}_3 = \delta \hat{h}$ is at the computational boundary, $\hat{x}_3 = 0.095$ is just after the “spurious peak” in the $\beta = \gamma = 50$ result, and $\hat{x}_3 = 0.4$ corresponds to a height in the outer layer. The simulations are the same as those presented in §5.3.3, i.e., $\alpha = 2$ and $C_S = 0.1$ were used. In Figure 5.16 a turbulent plane at $\hat{x}_3 = 0.1$ from the DNS Re$_\tau \approx 1000$ study by Cimarelli et al. (2015) is plotted for comparison.

At $\hat{x}_3 = \delta \hat{h}$ we can confirm the increase in variance of the turbulence fluctuations for the $\gamma = -5$ case against $\gamma = 50$ that was observed in Figure 5.9. The addition of a $\gamma$ boundary condition gives a variation that is approximately twice that of the $\gamma = 50$ case at the boundary. When the spurious peak is passed, illustrated here at the level $\hat{x}_3 = 0.096$, the turbulent fields of the two cases are more similar; whereas the $\gamma = -5$ structures are slightly less “streaky” in nature. Compared to the DNS result the shape of the resolved structures are of reasonably shape. Further out, as illustrated at $\hat{x}_3 = 0.4$, no differences in the turbulence can be noticed between the $\gamma = -5$ and 50 cases anymore.
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Figure 5.15: Instantaneous horizontal planes $(x_1, x_2) \in [0, 4\pi] \times [0, 2\pi]$ of the $(\bar{u}_1 - \langle \bar{u}_1 \rangle)/u_\tau$ field at the final time of the simulations. A comparison of the results computed with slip boundary conditions $\beta = \gamma = 50$ (left column) and $\beta = 50$, $\gamma = -5$ (right column).

Figure 5.16: Similar as in Figure 5.15 but for from the DNS simulation of $Re_\tau = 1000$ by Cimarelli et al. (2015), taken at $\tilde{x} = 0.1$ and non-dimensionalized with a the centerline velocity. (left) DNS field. (right) Same field but low-pass filtered.
Numerical results

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Figure 5.17: (a) Streamwise mean velocity profiles; (b) relative error of the derivative to capture a logarithmic behavior. Result of different vertical resolutions for a fixed (grid independent) Smagorinsky length scale $l_S$.

5.3.6. Grid dependency

Using a spectral method with a Chebyshev grid point distribution in the vertical direction where the clustering of points cannot be linked to the size of the turbulent structures is a rather unusual setup for wall modeled LES. Except for the discussion about commutation errors etc. the filter width definition in the Smagorinsky model becomes rather unclear; different definitions will change the Smagorinsky length scale $l_S$ completely; see also §2.2.4.

Introducing a matching function means that we are fixing the Smagorinsky length-scale independently of grid-point distribution. Furthermore, the slip boundary conditions where we fix the friction coefficient parameters are also grid independent. The question now is, is it possible to separate the filter width definition of the Smagorinsky model from the actual grid resolution?

To study grid dependency we fix all parameters in the equations we are solving and refine the grid in a step-wise manner. In our case we need to fix the Smagorinsky length-scale $l_S(x_3)$. This means that the vertical filter width that previously were chosen as the maximal grid spacing in the vertical direction now must be chosen in an universal way. Without going into details in what the best universal choice is, we chose $\delta_{\max}$ equal to that of the $N_3 = 65$ resolution for all the cases that are here studied. Since we are mainly interested in the vertical grid point dependency we fix the horizontal resolution to $N_1 = N_2 = 64$ and change the vertical resolution as follows: $N_{x_3} \in \{25, 33, 49, 65, 73, 81\}$. We furthermore also fix the time step size to $\delta t = 0.005$ time units which gives stable results for all the $N_3$ just presented (for higher $N_3$ a smaller $\delta t$ is needed.
due to the explicit time discretization). For the rest of the parameters we picked $\beta = 20$, $\gamma = -5$, $C_S = 0.1$.

In Figure 5.17 we plot the streamwise velocity profiles for the cases above and the relative error of the vertical derivative (similar to many of the earlier Figures in this section). We can note that the results by two coarse resolutions $N_3 = 25$ and 33 deviate from the rest but that the results of the remaining resolutions do not differ much from each other. In line with the previous studies in this chapter we furthermore plot the streamwise turbulence intensity; see Figure 5.18. Here we can see a slight variation of the results of also the moderate resolutions, however the differences are rather minor.

5.3.7. Summary

In this section we solved the filtered Navier stokes equations in an open channel domain. The standard Smagorinsky model was employed and the Reynolds number was assumed so high that all the viscous effects could be included in the eddy-viscosity part. The setup can be seen as the simplest form of a neutral atmospheric boundary layer. As a wall model to bypass the viscous wall region partial slip boundary conditions were employed together with a mixing length matching function.

For the slip boundary conditions the new approach of imposing different friction coefficients on the zero and non-zero wavenumber boundary conditions was assessed successfully. The well known spurious peak in the streamwise turbulence intensity could be eliminated through the changes in the boundary conditions. We furthermore showed the importance in using a stress matching function to get a robust result and to obtain wanted logarithmic behavior at
the wall-modeled boundary. We can conclude that a “wall model” is really a combination of appropriate wall boundary conditions together with appropriate SGS modeling in the near wall region. Finally a grid dependency study was carried out which further strengthened the evidence in the great robustness of the near wall model and the matching function approach.

5.4. Preliminary results for LES of stably stratified flows

During night-time an atmospheric boundary layer is generally stable. Cooler air at the Earth’s surface leads to a potential-temperature profile that has a positive gradient which generates negative vertical buoyancy forces which act as a turbulence destruction mechanism. The mean velocity profile gets modified due to the buoyancy which can be explained by the fact that the horizontal Reynolds stresses \( \langle u'_j u'_3 \rangle \), \( j = 1, 2 \), get smaller. Thus, close to a smooth wall where the viscous stress is dominating the profile is less affected by the buoyancy than further out in the boundary layer where the Reynolds stress becomes demanding; the differences against the neutral case becomes here more pronounced. Furthermore, when the buoyancy becomes too strong, turbulence cannot longer sustain and the flow typically relaminarize.

In this section we consider a few simulations of stably stratified flows. We solve the filtered Navier–Stokes equations with the Boussinesq approximation applied as discussed in §2.19 over the non-dimensional domain \( \Omega \), given in (5.1). We start presenting low Reynolds number wall resolved LES, and move on to high Reynolds number simulations.

5.4.1. Low Reynolds number test cases

DNS of low Reynolds number stably-stratified channel flows of \( \text{Re}_\tau = 180 \) up to 550 were studied by García-Villalba & Del Alamo (2011) utilizing moderately high resolution. We start doing some initial validation to their results, performing low resolution LES (64\(^2\)×65 grid points) with the modified Smagorinsky model (Equation 2.27) together with a van Driest wall damping function (Equation 3.32) for the eddy-viscosity at both the upper and lower boundaries. Different strengths of stratification were chosen as viscous scaled Richardson numbers \( \text{Ri}_\tau := \text{Ri}/u_\tau^2 \in \{0, 18, 60, 120\} \) where \( \text{Ri} \) is the constant Richardson number used in the buoyancy term of the momentum equation. In order to obtain converged turbulent statistics for the higher stability cases the initial conditions were chosen as close to the final result as possible. Lower stratification results were used as initial conditions for stronger stability cases and under-resolved DNS were used as initial conditions for the LESs. For the scalar equation the initial condition of the first simulation was chosen as a linear profile from zero at the lower boundary up to one at the upper. Boundary conditions for the scalar were chosen as Dirichlet conditions consistent to the initial condition as zero and one. For the resolution employed it turned out that the Smagorinsky coefficient had to be chosen rather low for the flow to not laminarize. A Smagorinsky coefficient of \( C_S = 0.025 \) was used for all the
5.4. Preliminary results for LES of stably stratified flows

Figure 5.19: LES of stably stratified channel flows of $Re_{\tau} = 180$. (a) streamwise mean velocity profiles. (b) mean scalar profiles. (c) streamwise turbulence intensity. (d) modified Smagorinsky model factor.

results that are now presented. In all simulations the Prandtl number for the scalar equation was chosen as $Pr = 0.7$.

In Figure 5.19 the statistics of the lowest Reynolds number case $Re_{\tau} = 180$ is shown. We can see that with an increased stability the velocity profile outside the viscous wall region steepens more and more as a consequence of the less efficient Reynolds stress $\langle u_j' u_3' \rangle$ and that the profiles there become closer to a laminar parabolic profile. We can also see that the magnitude of the turbulence intensity close to the wall is not much affected by the stratification.

For the mean scalar statistics (see Figure 5.19b) we plotted $\langle \bar{\theta} \rangle / \theta_{\tau}$ where $\theta_{\tau} := \kappa \partial_3 \bar{\theta}|_{wall} / u_{\tau}$, with $\kappa = (RePr)^{-1}$. The effects of stratification are similar for the scalar as for the mean velocity; near the surface the buoyancy has very little influence and in the outer part the profiles steepens more and more with an increased stability.
5. Numerical results

Figure 5.20: Effect of the Smagorinsky model for the $Re = 180$ stably stratified simulation. Under resolved DNS (solid). Modified Smagorinsky LES (dotted) with $C_S = 0.025$.

Compared to the DNS results by García-Villalba & Del Alamo (2011) our statistics deviates slightly. For instance the turbulence intensity maxima (seen in Figure 5.19c) are slightly underestimated and the mean velocity is overall lower outside the viscous wall region. These deviations are likely to be fixed by using e.g. a larger Smagorinsky coefficient or a higher resolution. Recall, we used a very low Smagorinsky coefficient. In Figure 5.20 the LES is compared to the under-resolved DNS. An effect from the Smagorinsky model is obtained, but it is rather low. A higher resolution would be needed in order to use larger Smagorinsky coefficients without making the flow relaminarize.

In Figure 5.19d we plot the factor $T$ for the modified Smagorinsky model (2.27). It is clear that factor gets smaller as the local effect of stability becomes stronger. This is directly consistent with the definition (2.27), a higher $\partial_3 \bar{\theta}$ leads to a smaller $T$.

In Figure 5.21 we further show results computed with the higher Reynolds number $Re = 550$ for $Ri = 120$, included is also the $Re = 180$ result for comparison. For the $Re = 550$ case the resolution of 65 Chebyshev points in the vertical direction leads to three points below $x_3^+ = 5$ which should be enough to (roughly) resolve the viscous sublayer. In Figure 5.21a the mean streamwise velocity profiles are plotted. Increasing the Reynolds number leads to a thinner viscous sublayer and the mean velocity profile shows a more clear stratified behavior. Compared to DNS (see Figure 5.20a) the streamwise mean profile of the $Re = 550$ case also matches the DNS fairly well. Interestingly the mean profile of the $Re = 550$ case follows a logarithmic behavior up to approximately $x_3^+ = 100$ (see Figure 5.21c), then for higher $x_3^+$ the stable stratification takes over more and more. An increase in Reynolds number leads also to a change in the mean scalar profile; see Figure 5.21b. The gradient close to the wall, corresponding to a diffusive layer, gets steeper, and an inversion
5.4. Preliminary results for LES of stably stratified flows

![Graphs showing LES results](image)

Figure 5.21: LES of stably stratified channel flows of Re\(_\tau\) = 180 (dashed & ×) and Re\(_\tau\) = 550 (solid & o). In (a) the dotted line is the Re\(_\tau\) = 550 result by García-Villalba & Del Alamo (2011), and in (c) the dotted line is the Re\(_\tau\) ≈ 5200 result by Lee & Moser (2015).

in the middle of the domain becomes steeper as well. Moreover, as the scalar gradient gets steeper, the stratification becomes stronger and the modified Smagorinsky model factor \(T\) smaller; see Figure 5.21d.

5.4.2. High Reynolds number wall modeled LES

The low Reynolds number test cases presented above gave us a first indicator on the impact of the stratification in a wall bounded flow. We now move on to the more relevant model problem for atmospheric boundary layer flows.

The setup is here similar as for the neutral case in §5.3. We consider an open channel domain and we move the high Reynolds number dependency over to the eddy-viscosity by introducing an artificial viscosity (see §4.4). For the scalar, we similarly introduce an artificial diffusivity. Both these artificial constants were chosen as 1/1000.
In this study, we used for simplicity the same initial and boundary conditions on the scalar as for the DNS. Simulations were run similarly as for the DNS case starting from initial conditions taken from converged statistics of a simulation of lower stability.

As wall boundary conditions we use here the same partial slip and no penetration boundary conditions as for the neutral case (Equation §5.13). Arguments for using similar boundary conditions on neutral and stratified cases were discussed in §3.3.2. We can also note from Figure 5.21c that a logarithmic-law based boundary condition becomes justified at around $x^+ = 30$ for the $Re = 550$ case. For the Smagorinsky model we use $C_S = 0.1$ together with the mixing length matching function. For the scalar the turbulent Prandtl number were chosen as $Pr_{SGS} = 0.6$.

In Figure 5.22 we present the streamwise mean velocity profiles for three cases: the passive scalar case, a $Ri = 48.6$ and a $Ri = 130.2$. We can conclude that the slip boundary conditions do here relax the inner region as desired. Considering stability functions (see Figure 3.3) and the lower Reynolds number results, the mean flow behavior becomes well captured.

5.4.3. Summary and remarks

Stably stratified channel flows (open and full) were performed for different Richardson numbers and for both low and high Reynolds number LES. The results so far indicate that the scalar implementation is working and that slip boundary conditions can be used also for stably stratified simulations. This study is however only in an initial stage. Boundary conditions on scalar need also be considered and more testing of SGS models must be done. The DNS results were simulated using a very low Smagorinsky coefficient since the flow tended
to laminarize very easily. To do relevant simulations that do not laminarize we believe that higher resolution in the horizontal planes are also needed.
Chapter 6

Discussion and conclusions

In this thesis we have presented ideas about wall boundary conditions for LES of atmospheric boundary layers using partial-slip boundary conditions for which friction coefficients were derived from the standard logarithmic law as well as the attached eddy hypothesis. The boundary conditions were successfully implemented in a Fourier–Chebyshev spectral code based on the normal-velocity normal-vorticity formulation. The implementations have been well documented and tested for wall modeled LES of both neutral and stably stratified horizontally homogeneous flows.

In LES of atmospheric boundary layers one solves for the filtered velocity quantities $\bar{u}$ instead of the continuous $u$ on a relatively coarse grid. The governing equations are modified such that the effect of the unresolved eddies becomes modeled through an extra term in the equations, the so called subgrid scale (SGS) tensor. Typically, the filtering is implicit through the discretization method itself. However, boundary conditions must be imposed on the filtered quantities $\bar{u}$, not on $u$. For an ABL it is incorrect to impose no-slip boundary conditions on the filtered quantities for several reasons: (i) The velocity gradient in the vicinity of the wall becomes extremely high. The correct filtered velocity at the boundary becomes for a moderately dense grid larger than zero. (ii) The surface is generally rough, and roughness elements are typically smaller than the grid spacing. The average flow through the roughness elements is not zero. (iii) An constant coefficient eddy-viscosity model does not generally account for the effect of no-slip conditions and must typically be corrected in the viscous wall region by e.g. a van Driest wall damping. However, if the viscous wall region is under resolved such a damping cannot be employed.

Partial slip boundary conditions (Navier slip) are effective boundary conditions that can take into account mean surface effects through a modeling parameter (the friction coefficient). Such conditions have been used in the past for e.g. super-hydrophobic surfaces where roughness elements are small and under resolved by the mesh. Lately these slip models have also been tested on turbulent channel flows and we have here extended these to atmospheric flows.

To test the new implementation and wall modeling ideas several simulations were conducted, including a low to moderate Reynolds number full channel flow DNS, a high Reynolds number open channel flow LES and a high Reynolds
number stably stratified open channel flow LES. The DNS case acted as a first indicator to study the influence of the slip conditions on the viscous wall region and the two latter cases represent model problems for atmospheric boundary layer simulations. Several different parameter setups were used; friction coefficients were changed for both the zero and non-zero wavenumber boundary conditions, respectively. From the DNS results we could see a clear potential in the slip boundary conditions to be used as wall models. We could there conclude that a slip boundary condition to a higher extent influences the viscous wall region and has less impact on the logarithmic and the outer regions. A spanwise slip condition further induces an increase in turbulence intensity at the wall and makes the viscous wall region even less pronounced. From the high Reynolds number LES results we could with the boundary conditions on the mean (zero wavenumbers) obtain a perfect logarithmic behavior in the mean profile close to the wall boundary, and with the new boundary conditions on turbulence intensity (non-zero wavenumbers) we could eliminate the “spurious peak” in the streamwise turbulence intensity. To match the SGS model to the stress of the logarithmic law a mixing length matching function by Mason et al. was tested. The matching function fixes the Smagorinsky length scale at the boundary corresponding to the log-law in the mean and relaxes the grid dependency of the Smagorinsky model. An addition of the matching function improves the near wall result drastically and gives an overall more robust result. We can conclude that the wall modeling here is a combination of the choice of parameters in the wall boundary conditions together with the subgrid scale modeling in the near wall region. The slip boundary conditions seem according to our results work reasonably well; deviations from the logarithmic behavior and a typical spurious viscous layer effect are to a higher extent caused by the subgrid scale model which is responsible for the stress distribution away from the boundary.

The slip boundary conditions allow fluctuations at the computational boundary where they are imposed and they provides us with control over the slip velocity and stress through friction coefficients. Compared to the commonly used wall boundary conditions that are used in ABL codes (stress boundary conditions), the partial slip conditions have the advantage of having an analytical description and thus a good mathematical support and being grid independent. Furthermore, the idea we have shown of imposing boundary conditions on different wavenumbers that can control the near wall turbulence intensity is only possible with slip boundary conditions. The commonly used wall models for ABL, to impose Dirichlet boundary conditions on the shear stresses are both grid dependent and method specific. Little is known about their mathematical properties, which in addition had to be done in a discrete framework. The current Robin-type boundary conditions show a very good behavior in comparably simple flow configurations, where a departure from equilibrium conditions is minimal. It remains an important topic to study further how these conditions will behave in more involved situations, in particular when a log region cannot be assumed. In these situations, the comparison to the more
established boundary conditions based on the shear stress will be interesting to assess. In that sense, the present results should be viewed as a first step towards developing conditions that are formulated in a continuous way, and are discretized afterwards, as opposed to basing the boundary conditions on a specific discretization.

Chebyshev spectral methods have not been used for atmospheric boundary layer LES before to the author’s knowledge. A potential reason for this is that they are more cumbersome to work with, and that boundary conditions for these are typically hard to implement. However, we have in this thesis shown that for the normal-velocity normal-vorticity formulation it is indeed possible to impose more complicated boundary conditions in a rather simple way.

In wall modeled LES it may seem less clear whether a Chebyshev method is advantageous over, for instance, a fourth order finite differences discretization (which is also available in some ABL codes). We should stress here that there is always an advantage of using a spectral method in terms of numerical errors; numerical dissipation and dispersion errors can be assumed negligible for a spectral method whether they are a relevant issue in low order finite differences codes. For a spectral method all errors can be attributed to the modeling part whereas in finite differences models the modeling and numerical errors mix together. It is an advantage in having the knowledge that an actual change in the modeling can be linked to a change in the result and that the change in the result is not due to some implicit numerical effect that one has no control over. This is particularly important in an atmospheric code where there are no exact validation cases available, and the dependency of the SGS model becomes severe.

An obvious consequence of the Chebyshev method is the clustering of points close to the boundaries, at least if no mapping is used. It is well known that a non-uniform grid spacing in LES may be problematic for several reasons. For instance, the derivatives may not commute with the LES filter and it is also problematic with the definition of filter-width in a Smagorinsky model. However, we relaxed the grid dependency in our simulations through the mixing length matching function. Also a short grid dependency study was performed in which we fixed the modeling in the wall normal direction and changed the grid resolution. We could conclude that in the near wall region the grid-dependency is indeed not very strong despite the clustering and that the matching function seems to work fairly well.

Another important aspect is computational efficiency, and in general time-to-solution. In the future we are interested in large scale problems of flows over wind farms which certainly becomes very expensive. We checked the timings of both DNS and LES implementations and could see that in a DNS around 50% of the computation time is spent on the explicitly treated part (the non-linear term), whereas for LES over 80% is spent on the explicit computations (now both nonlinear and SGS terms). A dynamic Smagorinsky model was also added for comparison, where we could measure that approximately 90% is spent on
the explicit computations in that case. It is of an interest to see if there are ways to make the explicit part cheaper to compute.

Another interesting aspect that is also linked to the explicit part of the solver and LES is time-step requirements. Since we treat the LES eddy-viscosity term (which is a diffusive term) explicitly, the (explicit) Runge–Kutta method needs typically smaller time steps than in the DNS case in order to produce a numerically stable result. We already use an artificial viscosity for the treatment of large Reynolds numbers. It is of interest to see if it is possible to optimize the time-step dependency even further.

Regarding the slip boundary conditions there are also some possible follow up studies. Apart from testing the conditions in more complex flow situations as discussed above, one can also extend the formulations to include nonlinear aspects. For the current implementation we are restricted to linear boundary condition operators in physical space. Friction coefficients cannot so far be chosen space-dependent like they are for a non-uniform roughness over the surface plane. Non-linear boundary conditions like these should indeed be possible to implement but require that the boundary condition systems are combined between different wavenumbers through convolution sums. This is interesting to further investigate.

Another interesting follow up study is to consider transpiration boundary conditions. Boundary conditions on the vertical velocity gives a more direct effect of surface roughness. Furthermore, in order to remove the spurious viscous layer effect completely we believe that the resolved Reynolds stress cannot go to zero at the artificial boundary which is the case if a no-penetration boundary condition is used.

Finally, also different ways of imposing the actual conditions are worthwhile studying. The partial slip boundary conditions can be imposed in a finite/spectral element code through weak form like John et al. (2004); see also Appendix A. Such boundary conditions can take pressure variations into account which makes it possible to study e.g., atmospheric flows over hills.

The main goal of the work in this thesis was to make it possible to simulate atmospheric boundary layer flows using our Fourier–Chebyshev code. This goal has been successfully achieved. The new implementation and boundary conditions have been shown to work properly and to generate accurate results for a number of test cases. We see a great potential in using slip boundary conditions for atmospheric boundary layer flows. They give more control have better mathematical support and are more general than the stress boundary conditions. This thesis would be a step in the direction of more accurate atmospheric boundary layer simulations.
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Appendix A

Boundary condition implementation in weak form

Partial slip boundary conditions in the general form presented in §3.1 can easily be implemented in weak form. There are therefore great possibilities to use these using variational methods such as finite elements or spectral elements to simulate flows over complex non-flat surfaces.

Suppose we want to solve the filtered incompressible Navier–Stokes equations (2.18a)–(2.18b) using a variational method in a bounded domain $\Omega$ over the solid boundary $\Gamma \subset \partial \Omega$ were we want to impose the following boundary conditions:

$$ n \cdot \bar{u} = 0, \quad \beta \bar{u} \cdot \tau_j + n \cdot \sigma(\bar{u}, \bar{p}) \cdot \tau_j = 0, \quad j = 1, 2, \quad \text{on } \Gamma. \tag{A.1} $$

Here $\sigma(\bar{u}, p) := 2(\nu_0 + \nu_t)\nabla^s \bar{u} - \bar{p}I$.

Let $(\phi, \psi) = \int_\Omega \phi \cdot \psi \, d\Omega$ define the $L_2$ inner product. Define test/trial functional spaces as:

$$ V := \{ v \in H^1(\Omega)^3 : v \cdot n = 0 \text{ on } \partial \Omega \}, \tag{A.2} $$

$$ P := \{ \bar{p} \in L^2(\Omega) : \int_\Omega \bar{p} \, d\Omega = 0 \}. \tag{A.3} $$

where $H^1(\Omega)^3 \subset L^2(\Omega)^3$ is the Sobolev space of functions with first order distributional derivatives. The variational form of (2.18a)–(2.18b) reads: Find $\bar{u} \in V$ and $\bar{p} \in P$ such that

$$ (\partial_t \bar{u}, v) + (\bar{u} \cdot \nabla \bar{u}, v) - (\bar{p}, \nabla \cdot v) + (2[\nu + \nu_t] \nabla^s \bar{u}, \nabla^s v) $$

$$ = (f, v) + \int_\Gamma (2[\nu + \nu_t] \nabla^s \bar{u} - \bar{p}I) \cdot v \cdot n \, dS, \quad \forall v \in V, \tag{A.4} $$

$$ (\nabla \cdot \bar{u}, q) = 0, \quad \forall q \in P. \tag{A.5} $$

Where we used

$$ (2[\nu + \nu_t] \nabla^s \bar{u}, \nabla v) = ([\nu + \nu_t] \nabla^s \bar{u}, \nabla^s v) + ([\nu + \nu_t] \nabla^s \bar{u}^T, \nabla^s v^T) $$

$$ = ([\nu + \nu_t] \nabla^s \bar{u}, \nabla^s v) + ([\nu + \nu_t] \nabla^s \bar{u}, \nabla^s v^T) $$

$$ = (2[\nu + \nu_t] \nabla^s \bar{u}, \nabla^s v). $$
The test function $\mathbf{v}$ can be decomposed into orthogonal components $\mathbf{v} = \mathbf{v}_{\tau_1} + \mathbf{v}_{\tau_2} + \mathbf{v}_n$ where

$$
\mathbf{v}_{\tau_1} := (\mathbf{v} \cdot \boldsymbol{\tau}_1) \boldsymbol{\tau}_1 \quad \mathbf{v}_{\tau_2} := (\mathbf{v} \cdot \boldsymbol{\tau}_2) \boldsymbol{\tau}_2 \quad \mathbf{v}_n := (\mathbf{v} \cdot \mathbf{n}) \mathbf{n}.
$$

Then the surface integral in (A.4) can be rewritten as follows:

$$
\int_{\Gamma} \sigma(\bar{\mathbf{u}}, p) \cdot \mathbf{v} \cdot \mathbf{n} \, dS = \int_{\Gamma} \sigma(\bar{\mathbf{u}}, p) \cdot (\mathbf{v}_{\tau_1} + \mathbf{v}_{\tau_2} + \mathbf{v}_n) \cdot \mathbf{n} \, dS
$$

$$
= \int_{\Gamma} \sigma(\bar{\mathbf{u}}, p) \cdot (\mathbf{v} \cdot \boldsymbol{\tau}_1) \mathbf{\tau}_1 + (\mathbf{v} \cdot \boldsymbol{\tau}_2) \mathbf{\tau}_2 + (\mathbf{v} \cdot \mathbf{n}) \mathbf{n} \cdot \mathbf{n} \, dS
$$

$$
= \int_{\Gamma} (\mathbf{n} \cdot \sigma(\bar{\mathbf{u}}, p) \cdot \boldsymbol{\tau}_1)(\mathbf{v} \cdot \boldsymbol{\tau}_1) \, dS + \int_{\Gamma} (\mathbf{n} \cdot \sigma(\bar{\mathbf{u}}, p) \cdot \boldsymbol{\tau}_2)(\mathbf{v} \cdot \boldsymbol{\tau}_2) \, dS
$$

$$
= -\int_{\Gamma} \mathbf{\beta}_1 (\bar{\mathbf{u}} \cdot \boldsymbol{\tau}_1)(\mathbf{v} \cdot \boldsymbol{\tau}_1) \, dS - \int_{\Gamma} \mathbf{\beta}_2 (\bar{\mathbf{u}} \cdot \boldsymbol{\tau}_2)(\mathbf{v} \cdot \boldsymbol{\tau}_2) \, dS
$$

where $\mathbf{v}|_{\Gamma} \cdot \mathbf{n} = 0$ were used for the third equality.
Appendix B

Stability functions for non-neutral atmospheric boundary layers

In the inner layer of an atmospheric boundary layer one may assume that the dominant scales for the mean horizontal velocity $U$ and mean potential temperature $\Theta$ depend upon the following sets of parameters respectively

$$\left\{ u_\tau, x_3, \frac{\partial U}{\partial x_3}, \frac{g}{\Theta}, \langle u'_3 \theta' \rangle \right\} \quad \text{and} \quad \left\{ \theta_\tau, x_3, \frac{\partial \Theta}{\partial x_3}, \frac{g}{\Theta}, \langle u'_3 \theta' \rangle \right\}. \quad (B.1)$$

where $u'_3$ is the vertical velocity fluctuations, $\theta'$ the fluctuations of $\Theta$, $u_\tau$ the friction velocity, $\theta_\tau := -\langle u'_3 \theta' \rangle / u_\tau$ a turbulent temperature scale and $g$ the gravitational acceleration constant. By the Buckingham Pi theorem, these sets form each two non-dimensional groups

$$\left\{ \kappa x_3 \frac{\partial U}{\partial x_3} \frac{x_3}{L} \right\}, \quad \text{and} \quad \left\{ \kappa x_3 \frac{\partial \Theta}{\partial x_3} \frac{x_3}{L} \right\} \quad (B.2)$$

where

$$L := \frac{-u^3_\tau}{\kappa z \langle u'_3 \theta' \rangle} \quad (B.3)$$

is the Obukhov-length. Universal functions $\Phi_U(x_3/L)$ and $\Phi_\Theta(x_3/L)$ can now be defined that links the two groups in (B.2) together

$$\Phi_U(x_3/L) = \frac{\kappa x_3}{u_\tau} \frac{\partial U}{\partial x_3}, \quad \text{and} \quad \Phi_\Theta(x_3/L) = \frac{\kappa x_3}{\theta_\tau} \frac{\partial \Theta}{\partial x_3}. \quad (B.4)$$

Thus,

$$\frac{\partial U}{\partial x_3} = u_\tau \frac{\partial U}{\partial x_3}, \quad (B.5)$$

$$\frac{\partial \Theta}{\partial x_3} = \frac{\theta_\tau}{\kappa x_3} \Phi_\Theta(x_3/L). \quad (B.6)$$
B. Stability functions for non-neutral atmospheric boundary layers

B.0.1. Integral forms

Integrating (B.5) from \( h_r \) to \( x_3 \) yields

\[
U(x_3) = \frac{u_r}{\kappa} \int_{h_r}^{x_3} \frac{\Phi_U(\eta/L)}{\eta} \, d\eta
\]

\[
= \frac{u_r}{\kappa} \left[ \ln(x_3/h_r) - \int_{h_r}^{x_3} \frac{1 - \Phi_U(\eta/L)}{\eta} \, d\eta \right]
\]

\[
\left\{ \frac{d(\ln \eta)}{d\eta} = \frac{1}{\eta} \right\}
\]

\[
= \frac{u_r}{\kappa} \left[ \ln(x_3/h_r) - \int_{h_r}^{x_3} [1 - \Phi_U(\eta/L)] \, d(\ln(\eta)) \right]
\]

where the wind \( U \) is assumed to be zero at \( h_r \), i.e., \( U(h_r) = 0 \). Integrating (B.6) in a similar manner and one finally appears at

\[
U(x_3) = \frac{u_r}{\kappa} \left[ \ln(x_3/h_r) - \Psi_U(x_3/L) \right] \quad (B.7)
\]

\[
\Theta(x_3) - \Theta(h_r) = \frac{u_r}{\kappa} \left[ \ln(x_3/h_r) - \Psi_\Theta(x_3/L) \right] \quad (B.8)
\]

where

\[
\Psi_U(x_3/L) = \int_{0}^{x_3} [1 - \Phi_U(\eta/L)] \, d(\ln(\eta)) \approx \int_{h_r}^{x_3} [1 - \Phi_U(\eta/L)] \, d(\ln(\eta)) \quad (B.9)
\]

\[
\Psi_\Theta(x_3/L) = \int_{0}^{x_3} [1 - \Phi_\Theta(\eta/L)] \, d(\ln(\eta)) \approx \int_{h_r}^{x_3} [1 - \Phi_\Theta(\eta/L)] \, d(\ln(\eta)) \quad (B.10)
\]

Here the approximations of integration from zero instead from \( z_0 \) is applied to make the functions satisfy \( \Phi_U(0) = 0 \), and \( \Phi_\Theta(0) = 0 \) so that the neutral logarithmic expressions are matched.

B.0.2. Curve fitting from experiments

For moderate \( x_3/L \) observations suggests that (for more information see Garratt 1992)

\[
\Phi_U(x_3/L) = \begin{cases} 
[1 - \beta_{U,1} \frac{x_3}{L}]^{-1/4}, & -2 < x_3/L < 0 \\
1 + \beta_{U,2} \frac{x_3}{L}, & 0 \leq x_3/L < 1
\end{cases} \quad (B.11)
\]

\[
\Phi_\Theta(x_3/L) = \begin{cases} 
\alpha_{\Theta,1} \left[ 1 - \beta_{\Theta,1} \frac{x_3}{L} \right]^{-1/2}, & -2 < x_3/L < 0 \\
\alpha_{\Theta,2} + \beta_{\Theta,2} \frac{x_3}{L}, & 0 \leq x_3/L < 1
\end{cases} \quad (B.12)
\]
where the constants $\alpha_{U,i}, \beta_{U,i}, \beta_{\Theta,i}$, $i = 1, 2$ have been fitted by several researchers. Probably the most used parameter values are those by Businger et al. (1971) measured at the Kansas fields in USA in 1968. The values of Businger are presented in table B.1 and also plotted in Figure B.1.

Table B.1: Parameter values for (B.11)-(B.12) by Businger et al. (1971).

<table>
<thead>
<tr>
<th>$\beta_{U,1}$</th>
<th>$\beta_{U,2}$</th>
<th>$\alpha_{\Theta,1}$</th>
<th>$\alpha_{\Theta,2}$</th>
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<td>4.7</td>
<td>0.74</td>
<td>0.74</td>
<td>9</td>
<td>4.7</td>
</tr>
</tbody>
</table>

Figure B.1: Graphs of the universal functions (B.11)–(B.12) for the parameters in table B.1.

Applying the universal functions (B.11)–(B.12) to the integrals (B.9)–(B.10) yields after some manipulation

\[
\Psi_U(x_3/L) = \begin{cases} 
2 \ln \left[ \frac{1}{2} \left( 1 + \frac{1}{\Phi_U(x_3/L)} \right) \left( 1 + \frac{1}{\Phi_U(x_3/L)^2} \right) \right], & -2 < x_3/L < 0, \\
-2 \arctan \left( \frac{1}{\Phi_U(x_3/L)} \right) + \pi/2, & 0 \leq x_3/L < 1 \\
-\beta_{U,2} z/L, & \text{otherwise}
\end{cases}
\]

(B.13)

\[
\Psi_{\Theta}(x_3/L) = \begin{cases} 
2 \ln \left[ \frac{1}{2} \left( 1 + \frac{1}{\Phi_{\Theta}(x_3/L)} \right) \right], & -2 < x_3/L < 0, \\
-\beta_{\Theta,2} x_3/L, & 0 \leq x_3/L < 1
\end{cases}
\]

(B.14)