MULTISCALE AND TURBULENT INTERACTIONS FOR URBAN MICROCLIMATE PREDICTION

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presented by

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Cover: Vertical velocity fluctuations (from $-2 \text{ m/s}$ to $2 \text{ m/s}$) plotted above the Hönggerberg Hill, at 200 m above ground level.

ABSTRACT

The interaction between the Atmospheric Boundary Layer (ABL) and the flow field in urbanized area is the source of several types of microclimate specific to cities. The urban heat island effect and the smog are two examples of such type of urban microclimate. The interaction between the ABL and the urban flow covers a wide range of scales. The large turbulent structures in the ABL have a typical size from 100 m to 1000 m. The turbulent structures near the ground generated by buildings have a typical size from 1 m to 10 m. Simulating such large range of scales covering one to two order of magnitude would be hardly feasible with a single domain Large Eddy Simulation (LES) model. To overcome this limitation, a nesting procedure LES-to-LES is proposed. A Small scale LES (S-LES) is embedded into a Large scale LES (L-LES). The L-LES model is dedicated to resolve the large turbulent structures of the ABL, while the S-LES model resolves only the small turbulent structures generated by the buildings. The one-way downscale coupling between both LES domains is achieved by interpolating the L-LES data on the coupled boundaries of the S-LES. To ensure numerical stability and a smooth transition between the L-LES and the S-LES fields, an implicit blending algorithm is introduced in the inner domain.

The nesting procedure is validated with a reference LES, which covers the same domain as the L-LES but with a refinement level of the S-LES. The S-LES is able to reproduce with great accuracy the mean flow, the Reynolds stresses and the spectra compared to the reference LES. The effects of the relaxation time, which controls the strength of the blending procedure, are investigated in detail. It is shown that the optimal relaxation time is proportional to the turbulent integral timescale.

A wind tunnel experiment is conducted in order to mimic multiscale interactions between the Convective Boundary Layer (CBL) and buildings. A CBL is generated from a finite area heated plate, with or without wall mounted cubes. The nesting procedure is able to reproduce most of the multiscale interaction between the CBL and
the wall mounted cubes. The large scale effects of buoyancy are under-estimated by the L-LES due to the limited grid resolution in the vertical direction and the sub-grid scale models.

The nesting procedure is finally applied to a realistic case. The S-LES domain includes the buildings of the ETHZ Hönggerberg campus. The L-LES domain extends over several square kilometers. The roughness elements are parametrized by a wall-model in the L-LES. A roughness layer generated by the buildings is predicted in the S-LES. This layer is two to three times higher than the mean building height and extends up to two kilometers downstream the Hönggerberg campus. The wall-model used in the L-LES is not able to predict with a reasonable accuracy such roughness layer, which can impact the quality of the results inside the S-LES.

The multiscale interactions in urban microclimate can be efficiently simulated by a nesting procedure. The S-LES is able to reproduce the majority of these interactions occurring in urbanized area. The quality of the nesting depends on the capabilities of the L-LES to give a good approximation of the parametrized elements. Two-way coupling and advance wall-model should be developed to further improve the S-LES results.
Les interactions multi-échelles entre la couche limite atmosphérique (ABL) et les écoulements de l’air en milieu urbain sont la source de plusieurs types de microclimat spécifique aux villes. Les îlots de Chaleur urbain (UHI) et le smog sont des cas typiques microclimats urbains. Ces interactions couvrent une large échelle de phénomène. Les plus grandes structures turbulentes dans l’ABL ont une taille qui varie de 100m à 1000m. Proche du sol, les structures turbulentes générées par les bâtiments ont une taille comprise entre 1m et 10m. Simuler une telle étendue d’échelles, couvrant un à deux ordres de grandeurs, est difficilement faisable avec une seule Simulation des Grandes Echelles (LES). Pour surmonter ce problème, une simulation imbriquée LES-dans-LES est proposée. Une LES des petites structures (S-LES) est imbriqué dans une LES des grandes structures (L-LES). La L-LES simule uniquement les grandes structures turbulentes de l’ABL, alors que la S-LES résout seulement les petites structures turbulentes créées par les bâtiments. Le couplage des grandes aux petites structures est fait en interpolant les valeurs venant de la L-LES sur les conditions aux limites de la S-LES. Pour s’assurer d’une bonne stabilité numérique et lisser la transition entre les résultats de la L-LES et la S-LES, une procédure implicite de mixage est introduite dans le domaine intérieur.

La procédure de simulation imbriquée est validée avec une LES de référence, qui utile the même domaine que la L-LES, mais avec une discrétisation spatiale similaire à celle utilisée dans la S-LES. Le S-LES est capable de reproduire avec une grande précision l’écoulement moyen, les contraintes de Reynolds ainsi que les spectres de turbulence en comparaison avec la LES de référence. Les effets du temps de relaxation, qui définit l’intensité de la procédure imbriquée, sont étudiés en détail. Il est montré que le temps de relaxation est proportionnel à la dimension temporelle turbulente (timescale).

Une expérience en soufflerie est faite de sort à recréer les interactions entre une couche limite convective (CBL) et des bâtiments. La CBL est générée par une surface chauffante d’une dimension finie, sur laquelle
une série de cube peut être montée. Une simulation imbriquée de ce modèle est capable de reproduire la plupart des interactions entre la CBL et les cubes. Les effets des grandes échelles de convection sont sous-estimés dans la L-LES à cause résolution du maillage dans la direction vertical et du modèle de sous-maillle.

La procédure imbriquée est finalement appliquée à un cas réel. Les bâtiments du campus de Hönggerberg de l’ETHZ sont simulés par la S-LES. La L-LES couvre un terrain de plusieurs kilomètres carrés. Les éléments rugueux dans la L-LES sont paramétrés par un modèle de surface. Une couche limite rugueuse générée par les bâtiments se crée dans la S-LES. Cette couche est deux à trois fois plus épaisse que la hauteur moyenne des bâtiments et s’étend jusqu’à deux kilomètres derrière le campus d’Hönggerberg. Le modèle de surface utilisé dans la L-LES n’est pas capable de prédire une couche limite rugueuse, ce qui a un impact sur la qualité des résultats dans la S-LES.

Les interactions multi-échelles dans un microclimat urbain peuvent être efficacement calculées par une simulation imbriquée. La S-LES est capable de reproduire la majorité de ces interactions. La qualité de la simulation imbriquée dépend de la capacité de la L-LES de produire une bonne approximation des éléments paramétrés. Un couplage bidirectionnel et des modèles de surface avancés pourraient améliorer les résultats dans la S-LES.
ACKNOWLEDGMENTS

The research presented in this thesis was done at the Laboratory of Multiscale Studies in Building Physics at EMPA, and at the Chair of Building Physics at ETHZ. Both labs are led by Prof. Jan Carmeliet.

First of all, I would like to thank Jan Carmeliet for giving me the opportunity to do my PhD in his group. I would also like to express my gratitude to Vikor Dorer, who was leading the urban physics group of the lab during my stay at EMPA. They both contribute to my PhD with their ideas and support. My Acknowledgments also go to the doctoral committee for their remarks, corrections and constructive critics toward the end of my thesis.

Multiple staff members of the lab had a profound impact on this thesis. I would like to give my warm thanks to Roger Vonbank who worked (battled?) several weeks to create the temperature measurement probe. This fine piece of engineering and electronics allowed me to perform high quality measurements in the wind tunnel. I cannot forget the great work of Beat Margelisch. He was always here to maintain the wind tunnel in a good working condition. He was also of a great help for the fabrication of my wind tunnel model and would like to thank him for letting me play with his tools in the wood shop. It was relaxing to build up some real stuffs from time to time. Finally, I would like to thank Martina Kock for her help in all the administrative tasks I had to performed during those three years.

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I would like to express my deep thanks to Marc Immer. Our multiple discussions on turbulent flows have greatly contribute to the quality of this thesis. He also introduced me to C++ and advanced

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programming concepts. The open source library we developed together strongly helped me in my research. I would also like to thank Marc for providing me the code of the turbulent inflow generator. Without it, the numerical part of this thesis would have not been possible.

The numerical simulations presented in this work are performed with OpenFOAM. I had the great opportunity to meet its creator, Prof. Hrvoje Jasak during the OpenFOAM winter school 2014 in Zagreb. His help in the development and the implementation of the nesting procedure in OpenFOAM was extremely valuable for my project.

I would like to thank Kelly Hess and Justin Strauss for the proof reading of my thesis. they certainly spent hours to track down and correct the multiple English mistakes I left in these lines.

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### NOTATION

#### FLUID DYNAMICS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>thermal diffusivity</td>
<td>$m^2 s^{-1}$</td>
</tr>
<tr>
<td>$\beta$</td>
<td>thermal expansion coefficient</td>
<td>$K^{-1}$</td>
</tr>
<tr>
<td>$C_p$</td>
<td>specific heat capacity</td>
<td>$J kg^{-1} K^{-1}$</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>timestep</td>
<td>s</td>
</tr>
<tr>
<td>$\Delta t_C$</td>
<td>wallclock time</td>
<td>s</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>molecular diffusivity</td>
<td>$m^2 s^{-1}$</td>
</tr>
<tr>
<td>$g$</td>
<td>gravity vector</td>
<td>$m s^{-2}$</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>wavenumber</td>
<td>$m^{-1}$</td>
</tr>
<tr>
<td>$f$</td>
<td>frequency</td>
<td>Hz</td>
</tr>
<tr>
<td>$k, TKE$</td>
<td>turbulent kinetic energy</td>
<td>$m^2 s^{-2}$</td>
</tr>
<tr>
<td>$k_{sgs}$</td>
<td>sub-grid scale turbulent kinetic energy</td>
<td>$m^2 s^{-2}$</td>
</tr>
<tr>
<td>$L_{ii,j}$</td>
<td>integral lengthscale in direction $i$ of component $j$</td>
<td>m</td>
</tr>
<tr>
<td>$\nu$</td>
<td>dynamic viscosity</td>
<td>$N s m^{-2}$</td>
</tr>
<tr>
<td>$p$</td>
<td>pressure</td>
<td>Pa</td>
</tr>
<tr>
<td>$p_k$</td>
<td>kinematic pressure</td>
<td>Pa</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandtl number</td>
<td>–</td>
</tr>
<tr>
<td>$Pr_t$</td>
<td>turbulent Prandtl number</td>
<td>–</td>
</tr>
<tr>
<td>$\mathcal{P}_k$</td>
<td>Turbulence production</td>
<td>$m^2 s^{-3}$</td>
</tr>
<tr>
<td>$\rho$</td>
<td>density</td>
<td>$kg m^{-3}$</td>
</tr>
<tr>
<td>$p_k$</td>
<td>kinematic density</td>
<td>$kg m^{-3}$</td>
</tr>
<tr>
<td>$S_{ij}$</td>
<td>stain-rate tensor</td>
<td>$s^{-1}$</td>
</tr>
<tr>
<td>$\Theta$</td>
<td>potential temperature</td>
<td>K</td>
</tr>
<tr>
<td>$T$</td>
<td>temperature</td>
<td>K</td>
</tr>
<tr>
<td>$t_i$</td>
<td>discrete time $i$</td>
<td>s</td>
</tr>
<tr>
<td>$T_{ii}$</td>
<td>integral timescale of component $i$</td>
<td>s</td>
</tr>
<tr>
<td>$u_i$</td>
<td>velocity component $i$</td>
<td>$m s^{-1}$</td>
</tr>
<tr>
<td>$z_0$</td>
<td>roughness length</td>
<td>m</td>
</tr>
<tr>
<td>$z_i$</td>
<td>height of the atmospheric boundary layer</td>
<td>m</td>
</tr>
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### Notation

#### Mathematic Operations and Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>$</td>
<td>a</td>
</tr>
<tr>
<td>$\langle a \rangle$</td>
<td>averaging operation on $a$</td>
</tr>
<tr>
<td>$a'$</td>
<td>fluctuating part of $a$</td>
</tr>
<tr>
<td>$\bar{a}$</td>
<td>filtering operation on $a$</td>
</tr>
<tr>
<td>$a''$</td>
<td>sub-grid scale part of $a$</td>
</tr>
<tr>
<td>$j$</td>
<td>imaginary number $j = \sqrt{-1}$</td>
</tr>
<tr>
<td>$\delta_{ij}$</td>
<td>Kronecker symbol</td>
</tr>
<tr>
<td>$\epsilon_{ijk}$</td>
<td>permutation symbol</td>
</tr>
</tbody>
</table>

#### Subscripts

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$</td>
<td>value of the first grid point above the surface</td>
</tr>
<tr>
<td>$i$, $j$, $k$</td>
<td>spatial directions according to the coordinate system</td>
</tr>
<tr>
<td>$s$</td>
<td>surface value</td>
</tr>
<tr>
<td>$sgs$</td>
<td>sub-grid scale</td>
</tr>
</tbody>
</table>

#### Superscripts

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L$</td>
<td>value from the large scale domain of a nested simulation</td>
</tr>
<tr>
<td>$R$</td>
<td>value from a reference simulation</td>
</tr>
<tr>
<td>$S$</td>
<td>value from the small scale domain of a nested simulation</td>
</tr>
<tr>
<td>Acronym</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>--------------------------------------------</td>
</tr>
<tr>
<td>ABL</td>
<td>Atmospheric Boundary Layer</td>
</tr>
<tr>
<td>AGL</td>
<td>Above Ground Level</td>
</tr>
<tr>
<td>AMSL</td>
<td>Above Mean Sea Level</td>
</tr>
<tr>
<td>CBL</td>
<td>Convective Boundary Layer</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>DES</td>
<td>Detached Eddy Simulation</td>
</tr>
<tr>
<td>DNS</td>
<td>Direct Numerical Simulation</td>
</tr>
<tr>
<td>F-LES</td>
<td>Flat plate LES</td>
</tr>
<tr>
<td>FVM</td>
<td>Finite Volume Method</td>
</tr>
<tr>
<td>HIE</td>
<td>Heat Island Effect</td>
</tr>
<tr>
<td>L-LES</td>
<td>Large scale LES</td>
</tr>
<tr>
<td>LDA</td>
<td>Laser Doppler Anemometry</td>
</tr>
<tr>
<td>LES</td>
<td>Large Eddy Simulation</td>
</tr>
<tr>
<td>M-O</td>
<td>Monin-Obukhov</td>
</tr>
<tr>
<td>NBL</td>
<td>Neutral Boundary Layer</td>
</tr>
<tr>
<td>NVD</td>
<td>Normalized Variable Diagram</td>
</tr>
<tr>
<td>NWP</td>
<td>Numerical Weather Prediction</td>
</tr>
<tr>
<td>PDE</td>
<td>Partial Differential Equation</td>
</tr>
<tr>
<td>PIV</td>
<td>Particle Image Velocimetry</td>
</tr>
<tr>
<td>R-LES</td>
<td>Reference LES</td>
</tr>
<tr>
<td>RANS</td>
<td>Reynolds Average Navier Stokes</td>
</tr>
<tr>
<td>Acronym</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>------------------------------</td>
</tr>
<tr>
<td>S-LES</td>
<td>Small scale LES</td>
</tr>
<tr>
<td>SBL</td>
<td>Stable Boundary Layer</td>
</tr>
<tr>
<td>sgs</td>
<td>sub-grid scale</td>
</tr>
<tr>
<td>TC-Fork</td>
<td>ThermoCouples Fork</td>
</tr>
<tr>
<td>TKE</td>
<td>Turbulent Kinetic Energy</td>
</tr>
<tr>
<td>UHI</td>
<td>Urban Heat Island</td>
</tr>
</tbody>
</table>
# CONTENTS

**ACKNOWLEDGMENTS** vii  
**NOTATION** ix  
**ACRONYMS** xi  

## 1 INTRODUCTION

1.1 Motivation ........................................ 1  
1.2 Scope and methodology .............................. 2  
1.3 Outline .......................................... 3  

## 2 BACKGROUND AND STATE OF THE ART

2.1 Fluid dynamics ..................................... 5  
  2.1.1 Turbulence ..................................... 6  
  2.1.2 Scales of turbulence ............................ 8  
  2.1.3 Statistical treatment of turbulence ............... 10  
2.2 Atmospheric boundary layer ......................... 15  
  2.2.1 Background .................................... 15  
  2.2.2 Research on ABL ................................. 22  
2.3 Nested simulation ................................... 25  
  2.3.1 Nesting in numerical weather prediction ........... 28  
  2.3.2 Nesting procedure for ABL ....................... 30  
2.4 Summary ........................................... 32  

## 3 GOVERNING EQUATIONS AND NUMERICAL MODELS

3.1 Conservation laws ................................... 35  
3.2 Turbulence modeling ................................ 38  
3.3 Large eddy simulation ................................ 39  
  3.3.1 Wall treatment for LES .......................... 43  
3.4 Reynolds Average Navier-Stokes ...................... 44  
3.5 One-way nesting for obstacles resolved LES .......... 45  
  3.5.1 Model equations ................................ 48  
  3.5.2 Model time stepping and algorithm ............... 49  
3.6 Wall-clock time evaluation .......................... 50  
3.7 Numerical solver ................................... 51  

## 4 NUMERICAL VALIDATION

4.1 Numerical model .................................... 53  
  4.1.1 Geometry and mesh .............................. 54
CONTENTS

4.1.2 Boundary conditions ................................................ 58
4.1.3 Turbulence model ................................................... 60
4.1.4 Solver parameters .................................................. 60
4.2 Effects of the blending zone ......................................... 61
4.3 Statistics ............................................................... 63
4.4 Spectra ................................................................. 68
4.5 Discussion ............................................................... 70
4.5.1 Effects and choice of the relaxation time ..................... 70
4.5.2 Seeding of synthetic small scale eddies ....................... 74
4.6 Transient scalar release ................................................ 75
4.6.1 Model setup and flushing procedure ......................... 75
4.6.2 Results and discussion ............................................ 78
4.7 Conclusions ............................................................. 84

5 EXPERIMENT VALIDATION .............................................. 87
5.1 Background .............................................................. 87
5.2 Experimental facility .................................................. 89
5.2.1 ETHZ/Empa Atmospheric Boundary Layer Wind Tunnel .................................................. 89
5.2.2 Particle image velocimetry ...................................... 90
5.2.3 Air temperature probe ........................................... 91
5.3 Model setup ............................................................. 93
5.4 Measurement protocol ................................................ 97
5.5 Wind tunnel results .................................................... 99
5.5.1 Flow statistics ...................................................... 99
5.5.2 Spectra and turbulent scales ................................... 107
5.6 Nested simulations ..................................................... 110
5.6.1 Domains and grids ................................................ 110
5.6.2 Boundary conditions and solver setup ...................... 114
5.6.3 Comparison with PIV, setup without cubes ............... 116
5.6.4 Comparison with PIV, setup with cubes ................... 120
5.6.5 Spectra from PIV and LES .................................... 129
5.7 Discussions and conclusions ...................................... 131

6 APPLICATION OF THE NESTED APPROACH TO A REAL CASE SCENARIO .................................................. 135
6.1 Topology and geometry ................................................. 136
6.2 model setup and boundary conditions ............................ 138
6.2.1 Outer domain ....................................................... 138
CONTENTS

6.2.2 Inner domain ................................................. 142
6.3 grid ................................................................. 143
6.4 Solver setup and nesting characteristics ................. 145
6.5 Generation of the inflow data ............................... 146
  6.5.1 Results .................................................. 148
6.6 Results ............................................................. 155
  6.6.1 Large scale LES ........................................ 155
  6.6.2 Small scale LES ......................................... 161
6.7 Discussion ......................................................... 167
6.8 Conclusion ......................................................... 170

7 CONCLUSIONS AND OUTLOOKS .......................... 171
  7.1 Synthesis ....................................................... 171
  7.2 Contributions to the research field ...................... 173
  7.3 Outlooks and perspectives ................................. 174

BIBLIOGRAPHY ......................................................... 177
INTRODUCTION

1.1 MOTIVATION

According to the United Nations (UN 2014) 66% of the world’s population will live in an urbanized area by 2050, which is more than doubled compared to 1950. The increasing size of urbanized areas also augments the effects on the local microclimate. One well-documented phenomenon is the Urban Heat Island (UHI) effect (Oke 1978; Stull 1988), which consists of rise in temperature in the urban areas compared to the rural surrounding (Fischer and Schär 2009; Schär et al. 2004). The UHI impacts the energy demand from the buildings (cooling and heating) and affects the health and the comfort of the population living in the city (Saneinejad 2013). Smog is another typical interaction between urbanized area and the local climate, where pollutants remain trapped in a city due to a stable atmosphere with weak mixing capabilities. Smog has become an important health risk in the recent decade.

The interaction between the microclimate and the urban wind flow covers a wide range of scales. Microscale phenomenon are responsible for hourly weather variations (see Figure 2.4 in Chapter 2), such as convective breezes, thunderstorms, and wake flows. Most of those effects take place in the Atmospheric Boundary Layer (ABL), which is the lower layer of the atmosphere directly influenced by the Earth surface. The ABL is mainly turbulent due the ground forcing (e.g. roughness and heat transfer) and topological features. The typical turbulent structures in the ABL spread from 100 m to 1000 m in size (Orlanski 1975; Stull 1988; Wyngaard 2010). Urban flows are also turbulent due to the interaction of the wind with the buildings and other roughness elements (lumps of forest, ponds, bridges). The size of the turbulence generated by these elements range between 1 m to 10 m. Those two ranges of scales are separated by one or two orders of magnitude. Solving such a wide range of scales in a single numerical model would be hardly feasible. One approach
to overcome this limitation is to use a multiscale simulation, where two or more numerical models are nested together. Each model is dedicated to resolve a specific range of scales. Two consecutive models are generally known as the outer and the inner model. The exchange of information between the two consecutive models is a critical aspect of such a nested simulation.

Operational mesoscale Numerical Weather Prediction (NWP) models cover a vast portion of terrain, from 500 km × 500 km up to 2000 km × 2000 km, with a horizontal resolution of 2 km to 15 km. The turbulence is generally modeled with the Reynolds Average Navier Stokes (RANS) approach, and the surface effects in the ABL are parametrized with complex wall-models. In some research mesoscale NWP models, the resolution is reduced down to 0.5 km, for a land cover of ≈ 100 km × 100 km. Despite having more cells near the ground, the ABL is still highly parametrized. Due to its turbulent nature, the flow in the ABL is generally simulated by a Large Eddy Simulation (LES). Typical ABL simulations cover several square kilometers (e.g. 10 × 10 km) with a spatial discretization down to 10 m, which is generally accepted as fine enough to resolve the typical ABL turbulent structures (Moeng 1984; Wyngaard 2010). Wind engineering LESs cover generally several hundreds of square meters, up to a few square kilometers. The grid resolution can go down below 30 cm in well-refined simulations. In a typical nested LES-to-LES simulation, an ABL-LES and a wind engineering LES are linked together. Nevertheless, this kind of coupling has not been clearly studied, and several open question remain, such as the transfer of information between the domains, the turbulence development within the inner LES and the influence of the parameterized elements in the outer domain which are geometrically resolved within the inner domain.

1.2 SCOPE AND METHODOLOGY

The goal of this thesis is to develop a nested LES-to-LES model, specifically designed to solve the multiscale interaction between ABL and urban flows. The outer LES solves the large ABL turbulent scales, whereas the inner LES is dedicated to the building-resolved urban flow. The information is transferred between the two models through
the nested boundaries of the inner LES. In order to smoothen the transition between the outer and the inner turbulent fields, an implicit blending procedure is applied inside the inner domain, in the vicinity of the coupled boundaries. The blending procedure allows the nested boundaries to be placed in regions with complex flow pattern.

The nesting and the blending procedure are validated against a reference LES, which covers the same domain of the outer LES but with the refinement level of the inner LES. A wind tunnel setup is designed to mimic the development of a Convective Boundary Layer (CBL) over a finite area heat surface. The measurements are used to validate the nesting procedure and to evaluate the capabilities of a nested-LES model in order to simulate large and small scale buoyancy. Finally The nesting procedure is used to simulate the interaction of a full size ABL developing over a realistic terrain and a cluster of buildings.

The nesting procedure is implemented in the Computational Fluid Dynamics (CFD) library OpenFOAM (Jasak 1996; OpenFOAM 2015). The new solver has been primarily designed for nested-LES, but any turbulence modeling approach can be used (LES or unsteady RANS). A new Python based library to post-process time-resolved LES and Particle Image Velocimetry (PIV) has also been developed (Vonlanthen and Immer 2015).

1.3 OUTLINE

This thesis is divided into seven chapters including this one, which presents the motivation for this thesis and the scope and methodology.

Chapter 2 presents the background knowledge of fluid dynamics and its application in microclimate predictions and wind engineering. The effects of turbulence on a ABL are presented in detail, as well as the statistical tools used to analyze turbulent flows. This chapter also includes a presentation of the state of the art research done in the fields of LES, ABL and nesting strategies.

The nested LES-to-LES model and the implicit blending procedure are presented in Chapter 3. To complete this chapter, the governing equations of fluid dynamics are included as well as a detail description of turbulence modeling with LES.
Chapter 4 presents the numerical validation of the nested procedure against a reference LES. The mean flow and higher order statistics are also compared. A spectral analysis of the flow is conducted to understand the development of fine-grained turbulent structures in the inner domain.

The wind tunnel setup is described in Chapter 5. The setup is reproduced for a nested-LES model and the numerical results are compared to the experiment.

In Chapter 6, the nesting procedure is used to simulate the flow through a cluster of buildings, under the influence of a CBL and a Neutral Boundary Layer (NBL). The buildings are built on a hill, that cannot be approximated by a flat terrain, therefore a nested-LES is used to include the evolution of the ABL over such a topology.

Finally, Chapter 7 gives the general conclusions of this thesis. Furthermore, an outlook is given to improve the reliability and the usability of the nesting procedure in realistic cases.
This chapter presents the relevant background knowledge of the motion of air in the atmosphere. As this thesis deals with the interaction between the atmosphere and urbanized areas, therefore a particular focus is put on explaining the phenomena involved in the lower part of the atmosphere, the so-called Atmospheric Boundary Layer (ABL). The nesting procedures used in weather prediction and wind engineering are presented in detail. They are the basis for the model proposed in this thesis in order to link the multiscale interaction between ABL flows and the flow around buildings structures.

### 2.1 Fluid Dynamics

Fluid dynamics has a huge number of applications in engineering, weather prediction, ocean current, geological flows, biology and more. This short list of applications gives an idea of the extremely wide range of scales covered by fluid dynamics, from the large atmospheric front to the microscopic flow in the capillaries of a human body. Furthermore, there are several classes of fluids with very different behavior, such as Newtonian, viscoelastic or viscoplastic. Among the fluids of a given class, their physical properties are subject to a large range of variation. For example, air, water and oil are all Newtonian fluids, but their density and viscosity are obviously very different.

The air composing the atmosphere can be described as a Newtonian fluid, where the viscous stresses are linearly proportional to the local strain of rate. Only two parameters are needed to describe the nature of the fluid: its density $\rho$ and its kinematic viscosity $\nu$. For every
time \( t \) and location \( x = [x_1, x_2, x_3] \) of an atmosphere flow, the velocity, pressure and temperature fields can be defined by

\[
\begin{align*}
\mathbf{u}(x, t) &= u_i(x, t) \\
p(x, t) &= p(x, t) \\
T(x, t) &= T(x, t)
\end{align*}
\] (2.1)

where \( i \in [1, 2, 3] \) are the components of the vector field \( \mathbf{u} \). Several other variables can be included to get a complete picture of atmospheric flows, such as moisture, concentration of various chemical components, fraction of water (liquid or gaseous), etc... The physical proprieties \( \rho \) and \( \nu \) of the air can also vary in space and time. Therefore they can also be considered as variables.

All those variables are dependent on the physical phenomena occurring in atmosphere. One of the most important phenomena taking place in the lower part of the atmosphere is turbulence. Due to its importance, it described in more detail in the following sections.

2.1.1 Turbulence

Any part of a flow is either laminar or turbulent. A laminar flow is characterized by its organization in layers without momentum convected between them. Mixing of heat, moisture and pollutants is only driven by physical diffusion. A turbulent flow has the following characteristics:

- **Chaotic**: Turbulent flows are characterized by their chaotic motion, even if it is known to be a deterministic process (by opposition to a random process), predicted by a set of deterministic equations. All the variables of a turbulent flow - velocity, temperature, scalars, moisture, etc - show a chaotic behavior. They are irregularly distributed in space and fluctuate in time. Moreover, Lorenz (1963) the father of the deterministic chaos theory, has shown that turbulent flows are strongly dependent on the initial condition, which makes detailed predictions extremely difficult. The turbulent quantities vary randomly from realization to realization.
• **Three dimensional and time dependent**: Turbulent flows are composed of three dimensional, chaotic structures named *eddy* or *vortex*. Those eddies are constantly created, transformed and dissipated into other smaller ones.

• **Mixing**: Turbulence has important mixing capabilities, in terms of momentum, temperature and passive scalar. It is several order of magnitude more effective than the physical diffusivity.

• **Dissipation**: Eddies are constantly transformed into smaller and smaller structures until they reach a size where the viscous dissipation becomes efficient and can convert the turbulent energy into heat. Without a production source, turbulence decays until it reaches a laminar state. This process in known as *relaminarization*.

Figure 2.1 shows the flow behind a hill in a water tunnel. Above the hill, the flow is laminar and organized in layers. In the wake of the hill, the flow field is turbulent. Notice the chaotic motion and the vortex-like structures in the shear layer between the laminar and the turbulent regions.

Figure 2.1: Flow behind a hill measured in a water tunnel. The water is charged with small air bubbles, which reflect the laser light sheet. From Van Dyke (1982).

Due to its chaotic behavior, turbulence has no analytic solution yet. It is still studied by means of observation and simulation. The first systematic and scientific studies of turbulence were conducted
by Reynolds (1883). In his work, he proposed the non-dimensional Reynolds number $Re$, which is used to classify a flow as turbulent or laminar. It reads as

$$Re = \frac{U_{ref} L_{ref}}{v}$$

(2.2)

where $U_{ref}$ is a reference velocity and $L_{ref}$ a reference length. Above a certain value of $Re$ the flow becomes turbulent. This transition does not occur at a fix value, because it strongly depends on the geometry and flow condition. In the beginning of the 20th century, Richardson (1922) proposed for the first time the concept of the turbulence cascade. This concept was further developed by Taylor (1935). It states that the largest eddies of a turbulent flow are the most energetic one. They break up into smaller and smaller structures with less and less energy. This can be seen as a cascade of scales and energy. In a second paper, Taylor (1938) proposed the concept of frozen turbulence. It defines an eddy as a frozen structure, which is convected downstream by the flow until it breaks up. This statement underlines the advection occurring in turbulent flow and the fact that eddies have a certain lifetime in the flow. This concept of frozen turbulence is quite accurate if the fluctuations are way smaller than the mean flow structures (Lumley 1965). Later on, Batchelor and Townsend (1948), Karman and Howarth (1938), and Lumley and Panofsky (1964) introduced some important concepts of the statistics to describe turbulence, especially on the properties of turbulent fluxes, both for engineering flow and geophysical flow. Kolmogorov (1942) proposed a theory on the distribution of turbulent energy across the turbulent cascade. He showed mathematically that the physics of the small eddies is independent of the studied case. In other words, the small turbulent structures are universal.

### 2.1.2 Scales of turbulence

As seen in the previous section, turbulent flows are composed of eddies of different sizes and energy content. Kolmogorov (1942) states that they are organized from the largest, high-energy to the smallest, low-energy eddies. The turbulent energy content can be plotted as a spectrum in function of the wave number $\kappa$. For a given turbulence flow and at sufficiently high Reynolds number, the turbulent energy spectrum $E(\kappa)$ has the typical shape shown in Figure 2.2. Toward the
small scales (large $\kappa$), the spectrum becomes universal. The organization from the high to the low energy wavelength is clearly visible

![Diagram of Idealized Turbulent Energy Spectrum](image)

**Figure 2.2:** Idealized turbulent energy spectrum and the three relevant regimes, $\mathcal{P}$, $\mathcal{T}$ and $\mathcal{E}$. Adapted from Pope (2000).

Several characteristic eddy sizes are highlighted in Figure 2.2. The largest possible eddies have the scale $L$, equivalent to the size of the geometry immersed in the flow. The turbulent structures with the size $L_I$ are located below them, which is known as the turbulent *length scale*. It is the size of the most energetic eddies in the flow. The structures characterized by those two scales are unstable, intermittent, anisotropic and case dependent. Turbulence is produced at those scales.

On the other side of the turbulent cascade, the smallest eddies have the characteristic size of $\eta = (\nu^3/\epsilon)^{1/4}$, and the time scale of $\tau_\eta = (\nu/\epsilon)^{1/2}$, where $\epsilon$ is the turbulent dissipation. $\eta$ and $\tau_\eta$ are called the Kolmogorov scales. On this scale, viscosity plays a major role and dissipates the turbulent energy into heat.

The size $l_{EI}$ and $l_{DI}$ are located between the production and the dissipation part of the cascade. They bound the energy transfer regime, where the turbulent energy is transported from the large to the small scale. Richardson (1922) is the first to identify this energy transfer, which is named *transition range* or *inertial subrange* nowadays. It was further formalized by Kolmogorov (1942) who showed that the
turbulent energy spectrum $E(\kappa)$ in the inertial subrange is proportional to:

$$E(\kappa) = C\epsilon^{2/3}\kappa^{-5/3}$$  \hspace{1cm} (2.3)

where $\kappa$ is the wave number and $C$ the Kolmogorov constant. This relation is known as the minus five-third law.

2.1.3 Statistical treatment of turbulence

The turbulence is time-dependent, chaotic and composed of eddies, or turbulent structures, organized by their energy and frequency. Therefore, statistics represents a good mathematical tool to analyze such physical phenomena.

Every turbulent scalar field $a(x,t)$ can be decomposed into a mean (or average) part and a fluctuating part:

$$a(x,t) = \langle a(x,t) \rangle + a'(x,t)$$  \hspace{1cm} (2.4)

where $\langle \cdot \rangle$ is the averaging operation and $a'(x,t)$ the fluctuation part of $a$. This decomposition is known as the Reynolds decomposition. This decomposition is used as a tool to analyze turbulent flows, and it is the basis for the widely used and well established Reynolds Average Navier Stokes (RANS) numerical method, which will be presented in more detail in Section 3.4.

Several averaging operations have been proposed in the history of turbulent study. Reynolds (1894) used the volume average, which holds only for homogeneous turbulence. Later the time average was introduced, which is more suitable for inhomogeneous flow and wall-bounded flows. Depending on the flow configuration, a modified versions of the volume and time average are used, such as surface averaging or moving time-averaging. Nevertheless, the most interesting method is the ensemble average introduced by Kolmogorov in the 1930’s. It can deal with any kind of flow, no matter if it is homogeneous or not, and steady state or not.
2.1.3.1 Mean and variances

An ensemble is a collection of $N$ independent realizations of a random turbulent field $a(x,t)$, obtained under identical conditions. The ensemble average is defined as the arithmetic average of the collection:

$$\langle a(x,t) \rangle_e = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} a(x,t:n)$$

where $a(x,t:n)$ is the $n$th realization of $a$. $\langle a(x,t) \rangle_e$ is called the expected value, or more commonly, the mean or the average. The mathematical operation of the ensemble average is shown in Figure 2.3. Despite its strength, the ensemble average is hardly usable in practice because it needs a large number of realizations (measurements or numerical results). If the process can be considered as ergodic over

![Figure 2.3: Example of an ensemble average on $N = 50$ realizations. Only the first four realizations are shown.](image)
a time window $\Delta t$, the ensemble average can be replaced by the *time average* defined as:

$$\langle a(x, t) \rangle_t = \frac{1}{\Delta t} \int_{t-\Delta t/2}^{t+\Delta t/2} a(x, t) \, dt$$  \hspace{1cm} (2.6)$$

Computing the time-average only requires one realization, therefore the vast majority of flow experiments and simulations are designed to be ergodic, hence *statistically stationary*. The statistical analysis presented in this thesis mostly uses the time-average operation. Therefore the subscript $t$ is removed to simplify the notation:

$$\langle a(x, t) \rangle = \langle a(x, t) \rangle_t$$  \hspace{1cm} (2.7)$$

The Reynolds average decomposition (Eq. 2.4) is applied to the velocity field $u$ gives

$$u_i(x, t) = \langle u_i(x, t) \rangle + u'_i(x, t)$$  \hspace{1cm} (2.8)$$

where $\langle u \rangle_i$ is the mean velocity field and $u'_i$ the velocity fluctuations. From the fluctuations, the covariance matrix, also known as the Reynolds stress tensor $\langle u'_i u'_j \rangle$, can be defined as

$$\text{cov}(u, u) = \langle u'_i u'_j \rangle = \begin{bmatrix}
\langle u'_1 u'_1 \rangle & \langle u'_1 u'_2 \rangle & \langle u'_1 u'_3 \rangle \\
\langle u'_2 u'_1 \rangle & \langle u'_2 u'_2 \rangle & \langle u'_2 u'_3 \rangle \\
\langle u'_3 u'_1 \rangle & \langle u'_3 u'_2 \rangle & \langle u'_3 u'_3 \rangle
\end{bmatrix}$$  \hspace{1cm} (2.9)$$

where the Einstein summation on $i$ and $j$ is used. The Einstein notation will be used as default notation in the rest of this thesis, except if specified differently. In the. By construction, $\langle u'_i u'_j \rangle$ is a symmetric tensor. The diagonal components $\langle u'_i u'_i \rangle$ are the variances of the velocity vector. When the Reynolds stress tensor is multiplied by the fluid density, each component $-\rho \langle u'_i u'_j \rangle$ can be seen as the mean force in the $i$-direction due to the fluctuation in the $j$-direction (Wyngaard 2010). With the diagonal elements of $Re$, the Turbulent Kinetic Energy (TKE) $k$ can be defined as

$$k = \frac{1}{2} \langle u'_i u'_i \rangle$$  \hspace{1cm} (2.10)$$

where the Einstein notation is used on the index $i$. 

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**BACKGROUND AND STATE OF THE ART**

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12
2.1 FLUID DYNAMICS

With the definition of the mean, the variance and the covariance, a proper definition of a stationary process can be formulated. A stochastic process like a turbulent flow is defined as stationary (or statistically stationary) if its probability distribution does not change in time. This has an important implication on the selection of the correct averaging method. As shown in Figure 2.3, the ensemble average can handle a non-stationary process without adding unwanted high-pass filter on the mean (the peak values are not smoothen out). The time-average can somehow deal with non-stationary processes by choosing the correct window, but the windowing always acts as a high-pass filter on the mean. The cutoff frequency depends on the window size and the window shape.

2.1.3.2 Correlation and spectra

The correlation $R_{ij}$ of velocity fluctuation time series $u'_i$ and $u'_j$, sampled at location $x_1$ and $x_2$, and at time $t_1$ and $t_2$ is defined as

$$R_{ij}(x_1,t_1,x_2,t_2) = \langle u'_i(x_1,t_1)u'_j(x_2,t_2) \rangle$$ (2.11)

If $i = j$, $R_{ij}$ is called the autocorrelation and if $i \neq j$ it is known as the cross-correlation. For the correlations, the Einstein notation is not used. The normalized version of the correlation is called the correlation coefficient and is defined as

$$r_{ij} = \frac{R_{ij}}{\sqrt{R_{ii}R_{jj}}}$$ (2.12)

To clarify the notation, $(x_1, t_1)$ and $(x_2, t_2)$ have been dropped out. If the flow is stationary, the correlation function $R_i(\tau)$ can be defined as

$$R_i(\tau) = \langle u'_i(x,t)u'_i(x,t+\tau) \rangle$$ (2.13)

where $\tau$ is the time lag. Both time series are extracted at the same location $x = x_1 = x_2$. The correlation coefficient function is defined in a similar manner as the correlation function:

$$r_i(\tau) = \frac{R_i(\tau)}{\langle u^2_i(x,t) \rangle}$$ (2.14)
In the same fashion, the spatial correlation function $R_{ij}(r)$ is defined by using two velocity time series extracted at the locations $x_1$ and $x_2$ at time $t$. The distance between the two locations is defined as the spatial lag $r$. Therefore $x = x_1 = x_2 + r$. The spatial correlation function can be written as

$$R_{r,i}(r) = \langle u'_i(x,t)u'_i(x+r,t) \rangle$$  \hspace{0.5cm} (2.15)

The spatial correlation coefficient function is then defined as

$$r_{r,i}(r) = \frac{R_{i}(r)}{\sqrt{\langle u'_i^2(x,t) \rangle} \sqrt{\langle u'_i^2(x+r,t) \rangle}}.$$  \hspace{0.5cm} (2.16)

$R_{r,i}(r)$ and $r_{r,i}(r)$ are commonly known as the two-point correlation and correlation coefficient functions, as they use two velocity time series from two locations $x$ and $x + r$. Throughout this thesis, $r$ is mostly aligned with one of the principal directions $x_1$, $x_2$ or $x_3$.

The autocorrelation function is used to extract the integral timescale $T_I$ defined as

$$T_{Ii} = \int_{0}^{\infty} r_i(\tau) d\tau.$$  \hspace{0.5cm} (2.17)

For each velocity component $i$, a timescale can be defined. Each of those timescales $T_{Ii}$ can be interpreted as the turn-over time of the most energetic eddies of a turbulent flow, in the direction $i$.

The two-point correlation functions is used to calculate the integral lengthscale $L_I$, which reads as

$$L_{Ir,i} = \int_{0}^{\infty} r_{r,i}(r) dr.$$  \hspace{0.5cm} (2.18)

By combining the three velocity components and the three spatial directions, nine lengthscales can be defined. The length scale $L_{Ii,j}$ can be seen as the dimension in direction $x_i$ of the most energetic eddies of the velocity component $u_j$.

The integral timescale is computed from a time-resolved point probe, which is quite easy to get, either experimentally or in simulation. The integral lengthscale needs time-resolved point-like data at several locations in direction $r$ to construct the $r_{r,i}$ function. Moreover the flow must be sufficiently homogeneous in this particular direction.
Those requirements make the lengthscale difficult to compute. Nevertheless, the lengthscales \( L_{ls,i} \) with \( s \) the streamwise direction, can be computed from the timescale by applying the Frozen turbulent hypothesis:

\[
L_{ls,i} = T_{li} u_s
\]  

(2.19)

where \( u_s \) is the velocity in direction \( s \). In a similar fashion, the autocorrelation function \( R_l(\tau) \) can also be converted in the spatial correlation \( R_{ss,i} \) by applying the Frozen turbulence with the velocity vector \( u_{ss} \).

The turbulent energy spectral density \( E_{ii}(f) \) of the velocity component \( u_i \) in function of the frequency \( f \) is defined as

\[
E_{ii}(f) = \left| \mathcal{F}(u_i) \right|^2 = \left| \int_{-\infty}^{+\infty} u_i(t) e^{-jft} dt \right|^2
\]  

(2.20)

where \( \mathcal{F}(u_i) \) is the Fourier transform of \( u_i \), \( \cdot \) the norm operator and \( j = \sqrt{-1} \) the complex number. \( E_{ii}(f) \) can also be computed from the Fourier transform of the autocorrelation function:

\[
E_{ii}(f) = \mathcal{F}(R_{ii}) = \int_{-\infty}^{+\infty} R_{ii}(\tau) e^{-jft} d\tau
\]  

(2.21)

Often, the turbulent energy spectrum is given in function of the wavenumber \( \kappa \), which gives direct information of the energy content of the eddies, depending on their size. It is defined as

\[
E_{ii}(\kappa) = \mathcal{F}(R_{r,i}) = \int_{-\infty}^{+\infty} R_{r,i}(r) e^{-j\kappa r} dr
\]  

(2.22)

2.2 ATOMIC ENERGY BOUNDARY LAYER

2.2.1 Background

Atmospheric flows are responsible for the weekly weather variations (alternation of high and low pressure fronts). They occur in the troposphere, which extends from the ground to roughly 11 km above sea level. The two features that distinguish atmospheric flow from other areas of fluid dynamics are the vertical density stratification of the medium and the Coriolis force due to the rotation of the earth. The
latter is responsible for new effects, which does not exist in laboratory, such as the dominant flow aligned with the line of isopressure and not with the pressure gradients. The Ekman spiral (Ekman 1905), which induces a rotation of the mean wind direction with the elevation is a typical phenomenon due to the Coriolis force.

Atmospheric processes are often classified according to their timescale and horizontal extend. As shown in Figure 2.4, atmospheric flows cover several order of magnitude in space and time.

![Figure 2.4: The scales of the atmosphere according Orlanski (1975) and further updated by Schlünzen et al. (2011). The horizontal and vertical axis represent respectively the typical timescale and lengthscale of the atmospheric processes. The gray boxes show the accepted naming convention for those scales.](image)

The atmospheric flow in the troposphere can be divided in two parts, the Atmospheric Boundary Layer (ABL) in the lowest 300m to 3000m and the free atmosphere up to the tropopause (Stull 1988). The
ABL is defined as the lower layer of the atmosphere, which is directly influenced by the earth surface. Its responds to surface forcing in about one hour or less in time and one kilometer or less in space. It is also subject to strong diurnal variation of temperature. The free atmosphere on the contrary shows little influence from the ground and from the day-night cycle. It is mainly driven by macroscale effect of the pressure, like depressions and fronts, and the temperature, such as cold or warm masses of air. According the classification of Figure 2.4, most of the effects taking place in the ABL are part of the microscale $\alpha$, $\beta$ and $\gamma$, with some of them extending in the mesoscale $\gamma$, such as sea breeze, urban heat island effect or deep convection.

The ABL is almost always turbulent. The two main sources of turbulent forcing are the surface friction, which always generates turbulent energy, and the heat exchange with the ground, which can be a source of turbulence if the surface is warmer than the air aloft, or a sink of turbulence in case of colder surface than the atmosphere. In term of turbulent scales, the energy containing eddies in the ABL have a typical size of $L_I = 10^2 \text{m}$ and can extend up to $L_I = z_i$, the height of the ABL. The inertial subrange extends from $l_{DI} = 10^2 \text{m}$ to $l_{EI} = 10^0 \text{m}$. Finally, the dissipative range stands around $\eta = 10^{-2} \text{m}$ (numbers according Wyngaard 2010).

Figure 2.5 shows the energy spectrum of the horizontal wind speed measured by Van der Hoven (1957). The peaks of the synoptic scales and daily cycle are clearly visible in timescales bigger than 10 h. The
low energy band between the mesoscale spectrum and the turbulent spectrum is known as the \textit{spectral gap}. The existence of the gap was further shown in various other studies, but in general the gap band is narrower and the energy peaks, especially the one of the turbulence, are lower and strongly influenced by the mean wind speed at the measurement time (Smedman-Högström and Högström 1974). The spectral gap extends from 5 min to 5 h. According Figure 2.4, it corresponds roughly to convective effects and thunderstorms. Despite being energetic weather features, they do not appear in the spectrum, because they are not regular enough events with a defined frequency, but more burst events. It must be noted, that the nature and the "size" of the spectral gap is still a matter of discussion in the scientific community.

The ABL can be divided in two parts, the \textit{inner layer} and the \textit{outer layer} as show in Figure 2.6. In the inner region, the flow is mainly driven by roughness elements such as buildings, patches of forest or civil engineering structures, and also by the surface roughness, like mature forests or cultivated fields. Here, the influence of the Coriolis force is not important in this layer. The outer region shows little dependence on the nature of the surface (buildings or forest) and the effects of the earth rotation begin to be relevant and an Ekman spiral can be visible. The interface between the two layers is not clearly defined. The overlapping region is known as the inertial sublayer.

![Figure 2.6: Schematics of the stable Atmospheric Boundary Layer (ABL). $z_i$ is the height of the ABL and $z_0$ the roughness length. Adapted from Garratt (1994) and Stull (2000).](image-url)
**ABLs** are classified according to their potential temperature $\Theta$ profile. The most common definition for $\Theta$ is:

$$\Theta = T \left( \frac{p_0}{p} \right)^{R/c_p}$$

(2.23)

where $T$ is the temperature, $p$ the pressure, $p_0$ the reference pressure, $R$ the gas constant and $c_p$ the specific heat capacity. The potential temperature is the temperature that a parcel of fluid at pressure $p$ would have if brought adiabatically at the reference pressure $p_0$. $\Theta$ is used to describe stratified flows because it removes apparent buoyant instabilities. For example, the pressure of a parcel of air decreases with the altitude and its volume increases. According to the perfect gas law (air can be seen as a perfect gas), its temperature will decrease, which leads to an apparent instability. Despite being stratified with cold air above warm air, the flow remains stable. Three types of **ABL** exist: the Convective Boundary Layer (CBL), the Stable Boundary Layer (SBL) and the Neutral Boundary Layer (NBL). Figure 2.7a shows the idealized velocity and potential temperature profiles of a CBL. It is in general topped by an inversion layer, or capping layer. The dashed lines shows the evolution of the profiles after a few hours. The CBL starts with a strong vertical temperature gradient. As the hours pass, the buoyant effects generate turbulences and vertical motions. They mix of the temperatures and increase the boundary layer height. The velocity is more evenly distributed with respect to the height, which increases its vertical gradient at the ground. In contrast, the SBL (Figure 2.7b) has poor mixing characteristics. The profiles do not evolve with time. As the ground is colder than the air aloft, the turbulence is damped and the boundary layer is shallower than the two other types of **ABL**. The NBL (Figure 2.7c) occurs mainly during periods of strong wind. In this case, the buoyancy has no effect on the turbulence, but the transfer of thermal energy still exists.
Figure 2.7: The idealized structure of the atmospheric boundary layer. The dashed profiles in a) and b) show the evolution of the profiles after several hours. The geostrophic line in the velocity charts show the theoretical wind profile without ground friction. Adapted from Stull (1988).
The diurnal temperature variation leads to a modification of the boundary layer structure as shown in Figure 2.8. In ideal conditions, a CBL develops during daytime, because of the warmer ground due to solar radiation. The top is often delimited by a thin, but strong inversion layer, or capping layer, with a thickness of 100 to 200 m and a temperature gradient of 2 to 5 °C per 100 m. At sunset, the short-wave radiation from the sun decreases and the ground cools down due to the emission of long-wave radiations to the space. A shallow SBL develops. The turbulence is damped and what remains of the CBL becomes the residual layer. The structure of the residual layer is not fully understood and its influence on the growing CBL just after the sunrise is not clear. It is still a topic of research nowadays.

Figure 2.8: Diurnal cycle of the idealized Atmospheric Boundary Layer (ABL). $z_i$ is the height of the ABL. Adapted from Stull (1988).

The flux Richardson number $R_i f$ is used in atmospheric science to define the turbulent state of the ABL. It is defined as

$$R_i f = \frac{\text{rate of buoyant destruction of TKE}}{\text{rate of shear production of TKE}} \quad (2.24)$$

which is represented in mathematical terms

$$R_i f = \frac{g}{\langle \Theta \rangle} \frac{\langle u'_3 \Theta' \rangle}{\langle u'_1 u'_3 \rangle} \frac{\partial \langle u_1 \rangle}{\partial x_3} \quad (2.25)$$

It depends on the covariance $\langle u'_3 \Theta' \rangle$, which can be seen as the mean vertical flux of the potential temperature fluctuation, and the turbulent shear-stress $\langle u'_1 u'_3 \rangle$, which is a term of the Reynolds stress tensor. For $R_i f < 0$ the atmosphere is unstable, for $R_i f = 0$ the flow is
neutral and for $Ri_f > 0$ stable conditions prevail. The flux Richardson number is well defined for all locations in the ABL. It requires all turbulent fluxes, which are difficult to measure in laboratory or during field experiments, or are not available in some types of numerical simulations, like RANS. Therefore, the gradient Richardson number $Ri_g$ is defined with the following relation:

$$Ri_g = \frac{g}{\langle \Theta \rangle} \left( \frac{\partial \langle \Theta \rangle}{\partial x_3} \right)^2 \left( \frac{\partial \langle u_1 \rangle}{\partial x_3} \right)^2$$ (2.26)

The gradient Richardson number is well defined at each point and requires only the mean gradient of temperature and velocity. If the gradients are not available, for example in a single point measurement, the bulk Richardson number $Ri_b$ proposes a simpler approach with

$$Ri_b = \frac{g}{\langle \Theta \rangle} \frac{\Delta \langle \Theta \rangle \Delta x_3}{\langle \Delta \langle u_1 \rangle \rangle^2}$$ (2.27)

The bulk Richardson number is mainly used to approximate the stability regime of the entire ABL.

2.2.2 Research on ABL

2.2.2.1 Homogenous and flat terrain

Most ABL studies are conducted on flat terrain with homogeneous land usage and roughness. Such idealized cases are more the exception than the rule in nature. Nevertheless, the assumption of horizontal homogeneity allows for theoretical analyses of the ABL vertical profiles. One of the most successful analysis is the Monin-Obukhov (M-O) similarity theory (Monin and Obukhov 1954). It describes the mean velocity and temperature profile of the ABL as a function of a dimensionless length parameter. The M-O similarity laws are explained in detailed in Stull (1988), Garratt (1994), and Kaimal and Finnigan (1993). Holtslag and Nieuwstadt (1986) proposed a review of the M-O laws and their applications for unstable and neutral boundary layers. They also emphasized their limitations in case of a stable ABL. Mahrt (1998) showed that the damping of turbulence in a SBL is the main issue for most of the similarity laws.
Despite the difficulty of finding a large enough flat terrain with homogeneous land usage, the velocity and Reynolds stress profiles have been measured in field studies with such topological configuration. The famous Kansas experiment (Haugen et al. 1971) provided the first extensive measurement of a convective ABL over a flat and homogeneous terrain. On the same experimental site, Kaimal (1973) analyzed the mean wind and temperature profiles, as well as the Reynolds stress, of a stratified boundary layer. To better understand the transition between the diurnal CBL and the nocturnal SBL, the SLTEST experiment has been conducted over a flat and smooth salt lake in the United States (Klewicki et al. 1998). The evolution of the temperature and wind profile was measured from the afternoon until midnight.

Lab experiments in a controlled environment provided further understanding of the of the convective boundary layer. Such experiments allow the full control of the boundary conditions (wall roughness and temperature, inlet profile). Deardorff et al. (1969) and Piper et al. (1995) conducted water convection tank experiments to understand the development of convective plumes in a stratified medium. To measure mixed convection, which is not possible in a convection tank, special boundary layer wind tunnels with controllable ground temperature (heated or cooled) are used. Moreover, the velocity and temperature profiles are adjustable at the inlet of the test section. Such fine pieces of hardware provide excellent tools to study several types of atmospheric boundary layers in detail. Fedorovich et al. (1996) and Ohya and Uchida (2004) measured CBL under a strong capping inversion. Ohya (2001) conducted a wind tunnel experiment for the SBL. He showed that there were two distinct flow regimes between the weakly and strongly stratified SBL flow. Under a critical Richardson number $R_i$, the destruction of turbulent structure due to the colder ground start to influence the mean flow field.

Large Eddy Simulation (LES) has been extensively used in atmospheric research to reproduce various boundary layer configurations. Deardorff (1970) proposed the first application of a LES for a convective boundary layer. From his simulations, he derived a new set of scaling laws for the mean velocity and temperature profile. In their paper, Moeng and Sullivan (1994) conducted several LESs in order to compare both a shear driven (neutral) and buoyant driven (unstable)
boundary layer. As the numerical solution resolves the full 3D field, they were able to clearly show the shape and the size of the turbulent structures. Several authors have also proposed combined wind tunnel and large eddy simulation studies. The wind tunnel is used as a validation for the simulation and the LES is used to complete the wind tunnel results with full field data. For example, Fedorovich et al. (2001) studied the development of a convective boundary layer under a capping inversion with wind tunnel measurements and LES calculations. Ohya and Uchida (2004) measured similar unstable ABL profiles and compared them to a Direct Numerical Simulation (DNS).

Neutral and unstable ABLs over homogeneous and flat terrain are rather well understood. Several high quality measurements and LES have validated the famous M-O similarity laws and proposed a new homogeneous model to explain the mixing in CBL. LES of ABL over homogeneous and flat terrain with cyclic side boundaries is a well established tool. Nevertheless, strong limitation arise from the use of cyclic conditions. Indeed, it is not possible to simulate land usage inhomogeneity and roughness resolved configurations.

SBL are more challenging to understand due to the opposite effects of the positive mechanical forcing and the negative buoyant forcing on the TKE. the M-O similarity laws do not hold in such configuration, and the few models proposed still show a lack of precision. As the turbulent structures in a SBL are much smaller than in a NBL or a CBL, the grid requirement of LES of SBL is very important. Therefore those simulations are limited to rather small horizontal extend.

2.2.2.2 Heterogeneous and realistic topography

Realistic topography and heterogeneous land usage (roughness, heat and moisture capacity) is the standard configuration of earth’s surface. The flow over complex terrain has very different features than its counterpart, over flat and homogeneous terrain. During daytime, thermal updrafts develop mainly on the sunny side of topologies. This leads to anabatic winds, flowing from the flat regions to the topographic elements (hills, mountains or valleys). During nighttime, the mean flow is reversed with the dense air moving toward the lower and flat areas. Despite such important differences, real terrains have not received the same attention compared to flat ones. Most of
the research has been performed on isolated and idealized topology features, like a single hill, periodic geometries like a repetition of 2D valley or even pattern of hills (Mason and Sykes 1979; Bradley 1980). The Askervein Hill Project is an example of a detailed field experiment on a isolated hill (Taylor and Teunissen 1987; Mickle et al. 1988). The wind speed, flow direction, temperature and Reynolds stress profiles were measured with several instrumented masts placed before, after and on the hill to provide a full set of measurements. Very recently, researchers have focused on so-called complex terrain, without periodic patterns. Whiteman (1990) conducted an extensive study of the mean flow and the local recirculation in valleys during the day and nighttime. Under the Mesoscale Alpine Program (MAP), Rotach et al. (2004) focused their measurements on the turbulent transport inside a steep alpine valley.

Due to the complexity of measurement campaigns on complex topology, numerical methods such as LES are very useful tools. They provide full 3D data, which helps to better understand complex turbulent structures. They also give insight into the flow high above the ground, where measurement masts are too short. For an isolated topographic feature, Golaz et al. (2009) did a LES on the Askervein Hill and compared his results with fields measurements cited in the previous paragraph. He was able to reproduce the mean velocity profile and the turbulent stresses with a quite good accuracy. Weigel et al. (2006a) and Weigel et al. (2006b) simulated the step valley topology covered by the MAP project (Rotach et al. 2004). The temperature and velocity profiles were correctly reproduced by the simulation, but turbulent fluxes show more discrepancies, especially near the ground in the valley.

2.3 Nested Simulation

A nested simulation is an unsteady Computational Fluid Dynamics (CFD) simulation composed of two domains: the outer and the inner one, also known as the large and small domain. The outer domain is filled with a coarse-grained grid with mean the grid dimension $\langle \Delta x^L \rangle$. The inner domain has a finer-grained grid compared to the outer one with a mean grid size $\langle \Delta x^S \rangle$. The superscripts $^L$ and $^S$ are used to
describe the elements (grid, fields, timestep, etc...) of the large and the small domain respectively. From the mean grid dimensions, the \textit{grid size ratio} is defined as

\[ N_{\Delta x} = \frac{\langle \Delta x^L \rangle}{\langle \Delta x^S \rangle}. \] (2.28)

\( \Delta t^L \) and \( \Delta t^S \) are the simulation timesteps for the outer and the inner domain respectively. The \textit{timestep ratio} is defined as

\[ N_{\Delta t} = \frac{\Delta t^L}{\Delta t^S}. \] (2.29)

Between the two domains, information needs to be exchanged. In a \textit{one-way} nesting procedure, the information is transferred only in one direction. In most of the cases, a \textit{one-way}, \textit{downscale} nesting is used, but \textit{one-way}, \textit{upscale} nesting is also possible. \textit{Two-way nesting} allows information to be transferred in both directions. For the downscale direction, the coarse-grained fields from the outer domain are interpolated at the boundaries of the inner grid. For the upscale direction, the fine-grained volumetric data are interpolated on the coarse grid. To get a smooth transition between the coarse and the fine-grained data, a blending procedure can be applied in the vicinity of the nested boundaries. The selection between a one-way or a two-way method depends on the type of coupling between the scales resolved by the inner and the outer domain.

Figure 2.9 shows an example of a nested simulation of the ABL above an urbanized area. It is composed of an inner \textit{LES} embedded in an outer \textit{LES}. The outer domain covers several km$^2$ of land and has a higher vertical extension than the mean ABL height. The coarse-grained grid is composed by cells with a size of 20 m, plus a level of refinement down to 10 m. Such cell sizes are quite common in CFD of ABL and are generally sufficient to capture all the energy-contained scale of a typical daily ABL. In this example, the buildings, shaded in gray, are not included in the domain. Their influence on the flow is parameterized. Depending on the case, they can be included in the domain, but they would be under-resolved\textsuperscript{1}. In this example the

\textsuperscript{1} in this context, under-resolved, means that the grid surrounding the structures would not be fine enough to properly capture all the physics. Well-resolved denotes the opposite situations.
inner domain covers only $1 \text{ km}^2$ of land and extends up to $0.5 \text{ km}$. The buildings are included in the simulation and resolved. The mean grid dimensions go from $4 \text{ m}$ to $2 \text{ m}$. With such grid resolution, the space between the buildings can be considered as relatively well-resolved, with exception of the walls. Figure 2.10 shows the same domain of interest, but instead, a LES with local mesh refinement is used.

In the example presented above, the inner domain can resolve smaller unsteady features compared to the outer one, therefore it
makes sense to select a timestep $\Delta t^S$ smaller than $\Delta t^L$. The ability to select a different timestep per domain is one of the main advantages of a nested simulation over a simulation with a locally refined mesh. The former allows a significant gain in computation time. In a CFD with a local grid refinement, the timestep has to be defined according to the smaller grid size. A lot of computational power is "lost" in the coarser grid cells by doing unnecessary timesteps. In a nested simulation, each domain is dedicated to a specific range of scales. Therefore the grid size and the time step is adapted to the scale to resolve.

The second advantage of a nesting strategy is the ability to activate different physics or models in each nested domain. For example, the turbulence modeling is likely to be modified when the driving mechanism of turbulence is substantially different. For example, the roughness model used in the outer domain can be changed or simply disabled in the inner domain if the roughness element are well resolved.

2.3.1 Nesting in numerical weather prediction

A nesting procedure in CFD can be applied to various situations where there is a clear separation of scales. Therefore it is a good approach to simulate atmospheric flows. It is used in production for Operational Numerical Weather Prediction (NWP).

Operational NWP models use highly specialized numerical solvers based on the RANS turbulent modeling. As atmospheric flows span over several orders of magnitude (see Figure 2.4), a computational domain is dedicated to each scale. In most cases, three domains are nested together with a one-way, downscaling method. Such nesting procedures are sometimes named RANS-to-RANS nesting. The largest domain simulates the macroscales $\alpha$, $\beta$ and up to some extend, the mesoscale $\alpha$. Generally, such model covers the entire earth with a horizontal grid resolution of 20 to 40km and between 50 to 100 layers in the vertical direction. The predictions are made on 15 to 30 days. The model one scale lower than the macroscale is known as the mesoscale model. It resolves the effects from the mesoscales $\alpha$, $\beta$ and sometime down to $\gamma$. The domain covers in general a continent with an horizontal grid resolution of 7 to 20km. The predictions are
generally made for 1 week in general. The smaller domain is known as mesoscale or microscale domain, depending on the grid resolution. It resolves the atmospheric effects from the mesoscale $\gamma$ to the microscale $\alpha$. Only a portion of continent surrounding the region of interest (a country for example) is covered by the domain. The typical horizontal cell size is 2 to 5km, with a trend toward 1km grid size. Two to three days prediction is the norm.

Figure 2.11 shows the nesting procedures used by the Met Office in United Kingdom and the Deutcher Wetterdienst in Germany. Both use their own in-house macroscale models. The UM$^2$ solver is used by the Met-Office for the two inner models. The smaller domain is nested to the mesoscale one with a one-way downscale procedure. The data from the mesoscale model are interpolated at its lateral boundaries. A blending procedure is added during the correction step of the numerical solver (see Davies 2013). The German office uses COSMO$^3$ for the medium and the small model. The nesting is done with the method proposed by Davies (1976). Again, a blending procedure is used in the vicinity of the nested boundaries.

Figure 2.11: Examples of nesting procedure used in operational NWP. (a) shows the nesting cascade adopted by the Met Office in UK and (b) by the Deutcher Wetterdienst in Germany. Illustrations from the website of the Met-Office (2014) and of the Deutsche-Wetterdienst (2014).

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2 Unified Model (UM)
3 Consortium for Small-Scale Modelling (COSMO)
2.3.2 Nesting procedure for ABL

In NWP, the trend is to increase the resolution of the inner most domain. Nowadays, most of the European meteorological offices are testing NWP models with a grid resolution down to 1 km or 0.5 km. But even with such spatial resolution, the NWP cannot resolve the typical turbulent features found in the ABL. Indeed, most of the operational NWP solvers are based on RANS models. The common RANS models (e.g. two equations models) strongly underestimate the anisotropy of the turbulent fluxes in a ABL. The vertical mixing in the CBL, a typical example the turbulence anisotropy, is weakly predicted and need some dedicated parametrization. LES models are good candidates to solve the problem of turbulence and anisotropy in ABL. As shown in the literature review in Section 2.2.2, LES models represent an excellent tool to model and analyze the turbulent processes involved in the ABL. Nevertheless, only a limited horizontal extend can be resolved with an average computational cluster: i.e. 3x3km to 10x10km. Therefore, nesting procedures involving one or two LESs are good candidate to solve this problem and it is studied for more than two decades. RANS-to-LES strategies are used to connect a microscale NWP to an ABL-LES. To resolve to even smaller scales, LES-to-LES nesting becomes interesting. In order to cover a wider range of scales, nesting cascades are possible.

Sullivan et al. (1996) were among the first to propose a one-way LES-to-LES nesting of the atmospheric boundary layer. The fine- and the coarse-grained domains have the same horizontal extension, but the inner one has a shallower vertical extend. The ground is flat and the land usage is homogeneous. Only the top boundary of the inner model is coupled to the outer one. With this configuration the flow statistics and the spectra are significantly improved near the ground and match well with the similarity laws. Moeng et al. (2007) investigated the two-way LES-to-LES nesting capabilities of the Weather Research and Forecasting (WRF) model to simulate an ABL (see Skamarock et al. 2005, for more detail on the WRF model). The inner model has a smaller horizontal extension than the outer one, but the same vertical dimension. The nesting is done via all the lateral boundaries. In comparison with a reference LES, the inner nested LES shows a mean temperature and a surface stress bias. According the
For terrain-resolved simulation, Golaz et al. (2009) proposed a one-way downscale LES nesting to simulate the flow over the Askervein Hill. He compared the numerical results with the well documented measurements done on the same topology by Taylor and Teunissen (1987) and Mickle et al. (1988). The hill is rather isolated from other topological features. The inner domain covers the hill plus a small extend of the flat surrounding. Due to the hill, standard cyclic boundary conditions can not be used. The outer domain has a flat terrain, where the cyclic approach is valid. The outer domain is simply used to provide realistic turbulent boundary conditions to the inner domain. The results from the inner LES agree well with the field experiments in terms of mean wind direction and intensity. The turbulent intensity is overestimated, especially above the top of the hill. According the authors, this is mainly due to the sgs model, not to the nesting itself.

Several authors used nested simulation to also resolve the flow around buildings. In the nesting, where more than two domains can be included, only the smallest ones are building resolved. Nozu et al. (2008) used a cascade of three nested LES to compute the pressure load on a building in downtown Tokyo. He also compared the numerical results with field measurements done on the same building. The pressure field of the inner-most domain reproduces the measured pressure distributions with a good accuracy, but the levels do not match the experiment. The author attributes these discrepancies mainly to the grid refinement and to the lack of measurements used to feed the boundary conditions of the outer-most domain. Nakayama et al. (2012) proposed a nesting cascade of NWP models followed by a nested LES to get the velocity field in downtown Tokyo during extreme events, like Typhoons and tropical storms. The main challenge in this case was to provide a turbulent inflow to the LES. Indeed, the coarse-grained field of the RANS model is not turbulent. Therefore fluctuations need to be reconstructed. This was done with a recycling method. The velocity profiles are reproduced with a very good accuracy compared to the large-scale WRF model. The gust factor, is somehow similar to observations, but the peak values from the LES are higher and shifted.
As highlighted in Section 2.3, one of the interests of a nested procedure is the possibility to use different models. Nozawa and Tamura (2010) proposed a one-way LES-to-LES nesting where the fine-grained domain solves the conservation equations for the fluctuation only. The coarse-grained domain solves the standard LES equations. With this configuration, the nested LES resolves only the missing eddies of the outer domain. To get the turbulent fields over all the scales, the data from the fine- and the coarse-grained grid are then summed up. This approach reproduces most of the turbulent structures with good accuracy. Nevertheless the nested boundary conditions of the inner domain are challenging to derive from the field of the outer simulation. The turbulent boundary fields have to be reconstructed somehow from the sgs-model.

2.4 SUMMARY

Nesting procedures have been first proposed for Numerical Weather Prediction (NWP) models to solve the multiscale arrangement of atmospheric structures (from large cyclones to local winds). In the field of RANS-NWP, nesting methods are well accepted. The same methods are applied to nested-LES to simulate an ideal Atmospheric Boundary Layer (ABL) (homogeneous flat terrain). Changing the turbulent model from a RANS to a LES is a profound modification. LES models are fully turbulent, with much smaller flow features than in RANS models. Moreover, those features are advected with the flow and transformed (energy cascade). Several of the previously cited studies have shown that nesting procedures develop for RANS-NWP can be applied for a flat surface ABL without too many disturbances. When the nested-LES is applied to a building-resolved geometry, the behavior of turbulence through the nesting is still unclear. For example, it is not known if the inner domain is able to recreate the fine-grained turbulent structures from the coarse-grained turbulent structures, especially in case of large nesting ratio. Furthermore, the inner domain of a building-resolved nested-LES needs to be able to handle complex inflow-outflow nested boundaries, as a purely inflow or outflow boundary hardly exists in dense urbanized area.
A LES nesting procedure, which can handle complex boundaries in urbanized area, is still missing.

In this thesis, a nesting procedure specifically designed to handle building-resolved nested-LES in a complex geometry is proposed. The procedure includes a blending zone to smoothen the transition from the coarse to the fine grained turbulent structures for any kind of nested boundary (inflow-outflow). The aim of the study is focused on the development of the proposed nesting procedure and a careful validation is conducted with a reference simulation and wind tunnel measurements. The possibilities of the method are studied in more detail in a realistic test case, simulating the interactions of a full scale ABL on a cluster of buildings.
GOVERNING EQUATIONS AND NUMERICAL MODELS

This chapter presents the governing equations and the numerical models used in fluid dynamics. As this thesis focuses on atmospheric flows, the equations are derived for air, but also remain true for a wider range of fluids. All the mathematical models in this chapter are presented in their final form, without the full derivation from the basic laws of conservation. More detailed discussions can be found in Ferziger and Peric (2002), Pope (2000) and Wyngaard (2010).

3.1 Conservation Laws

The air composing the atmosphere is a compressible medium. Its density changes with the altitude, the pressure and the temperature. Nevertheless, to simplify the formulation of the conservation laws and to make their numerical counterparts easier to solve, the flow is assumed incompressible. This hypothesis is true as the Mach number is always smaller than 0.3 in atmospheric flows. The conservation of mass and momentum for an incompressible flow can be written as:

\[
\frac{\partial u_i}{\partial x_i} = 0 \quad (3.1a)
\]

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = \frac{\partial \sigma_{ij}}{\partial x_j} \quad (3.1b)
\]

where the indices \(i,j \in [1,2,3]\) are the three spatial directions, \(t\) the time and \(\sigma_{ij}\) the stress tensor. Eq.3.1a and Eq.3.1b are written for the spatial direction \(x_i\). The left hand side of eq.3.1b is known as the material time derivative. The stress tensor represents all the forces acting
on a fluid particle. The air can be described as a Newtonian medium. With this hypothesis, the Eq. 3.1 can be rewritten as:

\[
\frac{\partial u_i}{\partial x_i} = 0 \quad (3.2a)
\]

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p_k}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \quad (3.2b)
\]

where \( u_i \) is the velocity in the direction \( i \), \( p \) the pressure, \( \rho \) the density and \( \nu \) the kinematic viscosity. The set of equations given by Eq. 3.2 is known as the Navier-Stokes equations for incompressible and isothermal flow. A full derivation of Eq. 3.2 can be found in Ferziger and Peric (2002, chapter 1).

Buoyancy is one of the main physical processes involved in the Atmospheric Boundary Layer (ABL). Buoyancy is driven by the local density changes due to temperature variations. But this is in contradiction with the incompressibility hypothesis. To keep this assumption valid, as it greatly simplifies the Navier-Stokes equations, the Boussinesq approximation for buoyancy is used. It assumes that the density fluctuation can be neglected except if the density is multiplied by the gravity. This hypothesis is widely used to simulate atmospheric flows and buoyant flow in general. A more formal justification of this assumption and its range of applications are given by Spiegel and Veronis 1960. The momentum equation with the Boussinesq approximation reads as:

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_0} \frac{\partial p_k}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \rho_k g_i \quad (3.3)
\]

where

\[
p_k = p + \rho_0 g_i h \quad (3.4)
\]

is the kinematic pressure and \( h \) the elevation, \( \rho_0 \) the reference density and \( g_i \) the gravity vector. The quantity \( \rho_k \) multiplying \( g_i \) in the last term of the right-hand side is the effective kinematic density. It takes into account small variations of density. If the variations of temperature remain small, it can be rewritten as:

\[
\rho_k = \frac{\rho}{\rho_0} = 1 - \beta(T - T_0) \quad (3.5)
\]
where \( T_0 \) is the reference temperature and \( \beta \) the thermal expansion coefficient. By combining Eq.3.5 in Eq.3.3, the conservation of momentum for an incompressible, Newtonian flow with buoyancy effect finally reduces to:

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_0} \frac{\partial p_k}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + (1 - \beta (T - T_0)) g_i \tag{3.6}
\]

To describe the atmospheric flow over large horizontal (several km) and vertical (deeper than the ABL) extends, the effect of the Coriolis forces must be added to the momentum equation. Below new term is added to Eq.3.6:

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p_k}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + (1 - \beta (T - T_0)) g_i + f_c \epsilon_{ijk} u_k \tag{3.7}
\]

where \( \epsilon_{ijk} \) is the permutation symbol, \( f_c = 2\Omega_e \sin(\phi_e) \) the Coriolis parameter, \( \Omega_e \) the angular speed of Earth and \( \phi_e \) the latitude.

In Eq.3.7 the temperature field \( T \) is a new unknown, which needs a new governing equation. The conservation of energy governs the evolution of temperature in the fluid. If the heat transfer in the flow is not affected by a phase change, chemical reactions, radiation and viscous effects, it can be written as

\[
\frac{\partial T}{\partial t} + u_j \frac{\partial T}{\partial x_j} = \alpha \frac{\partial^2 T}{\partial x_j \partial x_j} \tag{3.8}
\]

where

\[
\alpha = \frac{\nu}{Pr} \tag{3.9}
\]

is the thermal diffusivity and \( Pr \) the Prandtl’s number.

Throughout this thesis, the transport of a passive scalar \( s \) with the flow will be used several times. In this context, passive means that \( s \) does not interact with nor modify the flow field. The transport equation for \( s \) is defined as

\[
\frac{\partial s}{\partial t} + u_j \frac{\partial s}{\partial x_j} = \gamma \frac{\partial^2 s}{\partial x_j \partial x_j} \tag{3.10}
\]

where \( \gamma \) is the molecular diffusivity of the considered scalar. Eq.3.8 and Eq.3.10 are similar in form. In fact, in case of forced convection, the temperature can be considered as a passive scalar.
3.2 TURBULENCE MODELING

The Navier-Stokes equation (Eq. 3.2) can be used in a numerical solver to simulate any kind of flow. This approach is known as Direct Numerical Simulation (DNS). This implies that every scale and frequency must be resolved. In case of turbulent flow, this statement has some major implications. The scales involved in turbulence cover several orders of magnitude as shown in Figure 3.1 (logarithmic horizontal axis). For example in the Convective Boundary Layer (CBL), the energy-containing eddies have a length scale of \( L_i \approx 300 \text{ m} \). In the inertial sub-range, the eddies size extends from \( l_{DI} \approx 30 \text{ m} \) to \( l_{EI} \approx 3 \text{ cm} \). Finally, the dissipation occurs at sizes of \( \eta \approx 5 \text{ mm} \) (dimensions adapted from Wyngaard 2010). A DNS resolving all the scales of a typical CBL should have a grid composed of billions of cells with a size of roughly 1 mm\(^3\). This is beyond the computational power of any super-computer nowadays, and will remain like this for several decades. To overcome this issue, several turbulence modeling methods have been proposed. The two

![Idealized turbulent spectrum](image.png)

Figure 3.1: Idealized turbulent spectrum. Depending on the turbulence modelling (DNS, LES or RANS), the turbulence structures are resolved or modeled. Adapted from Pope (2000).
3.3 Large Eddy Simulation

The most prominent are the Large Eddy Simulation (LES) and Reynolds Average Navier Stokes (RANS) methods.

The LES method is based on the fact that the large scales $L$, $L_I$ and $l_{DI}$ are case specific and the small scales $l_{EI}$ and $\eta$ are universal. Therefore, it makes sense to resolve only the case specific scales and to model the other ones. This is done by applying a high-pass filter of width $\Delta$ to the turbulent fields (see Figure 3.1). This approach decreases the computational power by several orders of magnitude compared to DNS. Nevertheless, LES still remains a costly method.

The RANS method models all the scales (see Figure 3.1) by applying an ensemble average to the turbulent fields. Therefore, only the mean fields are resolved and the turbulence is modeled across the entire range of scales.

This thesis deals only with LES. Therefore, the method is presented in more detail in the following section. The RANS method is not used in this thesis, but is shortly presented in Section 3.4 as it brings some useful insights on the statistical treatment of turbulence. A complete presentation of the method is given by Pope (2000, chapter 11) and by Kundu et al. (2012, chapter 12).

3.3 Large Eddy Simulation

The spatial filtering operation of a space-time dependent turbulent field $a(x, t)$ is defined by the relation

$$\bar{a}(x, t) = \int_{-\infty}^{\infty} a(x') G(x - x') \, dx' , \quad (3.11)$$

which can also be written as

$$\bar{a} = G * a \quad (3.12)$$

where $G$ is the convolution kernel which characterizes the filter, $G *$ the filtering operation of $a$ by the kernel $G$ and $\bar{a}$ the filtered or resolved field $a$. One important parameter of $G$ is the filter width $\Delta$. It defines the region around $x'$ where the filtering is acting. $\Delta$ is also known as the window size. The unresolved part of $a$ is defined as

$$a'' = a - G * a \quad (3.13)$$
where \(a''\) is the unresolved or sub-grid scale (sgs) field of \(a\).

Applied to fluid mechanics, the filtering operation on the velocity \(u_i\) and the pressure \(p\) is defined as

\[
\overline{u}_i = u_i - u''_i \\
\overline{p} = p - p''
\]  (3.14a)

(3.14b)

where \(\overline{u}_i\) and \(\overline{p}\) are the filtered velocity and pressure respectively. \(u''_i\) and \(p''\) represent the sgs velocity and pressure. The filtered Navier-Stokes equations are derived from Eq. 3.2. A filtering operation is applied to Eq. 3.2 with \(p\) and \(u\) are replaced by their filtered counterpart of Eq. 3.14b and Eq. 3.14a:

\[
\frac{\partial \overline{u}_i}{\partial x_i} = 0
\]  (3.15a)

\[
\frac{\partial \overline{u}_i}{\partial t} + \overline{u}_j \frac{\partial \overline{u}_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \overline{p}}{\partial x_i} + \nu \frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}
\]  (3.15b)

with \(\tau_{ij}\) the sub-grid stress tensor defined as

\[
\tau_{ij} = \overline{u}_i \overline{u}_j - \overline{u}_i \overline{u}_j .
\]  (3.16)

The sub-grid stress tensor \(\tau_{ij}\) is symmetric by construction. It results from the filtering of the non-linear term \(\overline{u}_i \overline{u}_j\). It introduces six new unknowns in the system of equations 3.15. Therefore, it needs to be closed by adding six new equations or by applying a model. The transport equations for \(\tau_{ij}\) exist, but they again introduce new unknowns. Therefore \(\tau_{ij}\) is modeled by a so-called sgs turbulence model, or sgs model.

A large number of sgs models have been proposed. Most of them are based on the eddy viscosity model

\[
\tau_{ij} = \frac{2}{3} k_{sgs} + \nu_{sgs} S_{ij}
\]  (3.17)

with \(\nu_{sgs}\) the eddy viscosity,

\[
k_{sgs} = \frac{1}{2} \delta_{ij} \tau_{kk}
\]  (3.18)

the sgs kinetic energy and

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right)
\]  (3.19)
the resolved strain-rate tensor. The vast majority of sgs models are derived from the Smagorinsky model proposed by Smagorinsky (1963). It models $v_{sgs}$ as

$$v_{sgs} = (C_D \Delta)^2 |\mathbf{S}|$$

(3.20)

where $C_D$ is the Smagorinsky coefficient, $\Delta$ the filter size, and $|\mathbf{S}| = (2\bar{S}_{ij}\bar{S}_{ij})^2$ the magnitude of the strain-rate tensor $\bar{S}_{ij}$. Lilly (1967) proposed the following value for the Smagorinsky coefficient:

$$C_D \approx 0.17$$

(3.21)

which is correct for isotropic turbulence. In flow regions with high shear stresses or near the wall, this constant value is not valid anymore. It is also problem dependent and needs to be tuned with a priori data from a reference simulation or experiments. To overcome those problems, several authors have proposed *dynamic sgs models*. Instead of relying on a constant Smagorinsky coefficient, $C_D$ is constructed as a function of the local flow characteristic, such as the strain-rate tensor. Germano et al. (1990) proposed a dynamic $C_D$ coefficient based on the Germano identity (Germano et al. 1990; Germano 1992). It is valid for cases where the turbulence is homogeneous in one direction, like flows over a flat plate. Lilly (1992) improved on this model for general turbulent flows (without a specific homogeneous direction). The dynamic $C_D$ coefficient reads as:

$$C_D = \frac{1}{2} \frac{L_{ij}M_{ij}}{M_{ij}^2}$$

(3.22)

with

$$L_{ij} - \frac{1}{3} \delta_{ij}L_{kk} = 2C_D M_{ij}$$

(3.23a)

$$M_{ij} = \Delta^2 |\mathbf{S}| \bar{S}_{ij} - \Delta^2 |\mathbf{S}| \bar{S}_{ij}$$

(3.23b)

This model allows for realistic values of $C_D$ for anisotropic turbulence and wall bounded flow. This sgs model is known as the dynamic Smagorinsky-Lilly model. This model has demonstrated satisfactory results for ABL simulation under various stability regime (Kleissl et al. 2006; Stoll and Porté-Agel 2008; Langhans et al. 2012). Therefore this model will be used for all the LESs presented in this thesis.
If the numerical model includes other turbulent fields, their filtered counterpart needs to be included in their governing equation. The filtered temperature \( T \) is defined as

\[
\overline{T} = T - T''
\]

where \( T'' \) is the sub-grid scale temperature. By replacing \( T \) with \( \overline{T} + T'' \) in 3.8, the filtered equation of conservation of energy is defined as

\[
\frac{\partial \overline{T}}{\partial t} + \overline{u_j} \frac{\partial \overline{T}}{\partial x_j} = \alpha \frac{\partial^2 \overline{T}}{\partial x_j \partial x_j} - \frac{\partial q_i}{\partial x_j}
\]

where \( q_i \) is the \textit{sgs} heat flux. As for the conservation of momentum, the \textit{sgs} heat flux appears due to the non-linear term \( \overline{u_i T} \) in Eq. 3.8. It is modeled with the \textit{sgs} thermal diffusivity assumption, defined as

\[
q_i = \alpha_{s gs} \frac{\partial \overline{T}}{\partial x_i}
\]

where

\[
\alpha_{s gs} = \frac{\nu_{s gs}}{Pr_{s gs}}
\]

is the \textit{sgs} thermal diffusivity and \( Pr_{s gs} \) the \textit{sgs} Prandtl number. Few authors have proposed a \textit{sgs} model for \( Pr_{s gs} \) (Lilly 1992), but such advanced models are rarely used. Most of the LES proposed in literature use \( Pr_{s gs} = Pr_t \) as thermal turbulent model, with \( Pr_t \) the turbulent Prandtl number.

The transport equation of a filtered scalar \( \tilde{s} \) reads as

\[
\frac{\partial \tilde{s}}{\partial t} + \overline{u_j} \frac{\partial \tilde{s}}{\partial x_j} = \gamma \frac{\partial^2 \tilde{s}}{\partial x_j \partial x_j} - \frac{\partial u_i'' s''}{\partial x_j}
\]

where \( s'' \) is the sub-grid scale scalar and \( \gamma \) the scalar diffusivity. The \textit{sgs} scalar fluxes \( u_i'' s'' \) are treated like the \textit{sgs} heat flux, by introducing the \textit{sgs} scalar diffusivity:

\[
\overline{u_i'' s''} = \gamma_{s gs} \frac{\partial s''}{\partial x_i}
\]

with

\[
\gamma_{s gs} = \frac{\nu_{s gs}}{\gamma}
\]
3.3 Large eddy simulation

3.3.1 Wall treatment for LES

LES resolves only the energy containing eddies in a turbulent flow. Close to the ground, the energetic eddies become smaller and the velocity gradients increase. To properly capture the physics in this region, the grid resolution needs to be increased, which increases the computational cost drastically. Therefore a wall-resolved LES still remains limited to cases with a relatively low Reynolds number. A Reynolds number of several billion is common in atmospheric flows, therefore, wall-models for LES are needed.

Typical wall-models for LES prescribe the instantaneous shear-stress at the surface \( \sigma_{ij,s} \) with \( i,j \in [1,2] \) the streamwise and spanwise direction on the surface. Index \( s \) denotes values at the surface. The shear-stresses \( \sigma_{ij,s} \) are components of the stress tensor \( \sigma_{ij} \) (Eq. 3.1b). The model is introduced in the Navier-Stokes equation by splitting the right-hand side of Eq. 3.1b:

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = \frac{\partial \sigma_{ij,v}}{\partial x_j} + \frac{\partial \sigma_{ij,s}}{\partial x_j}
\] (3.31)

where the index \( v \) represents the values in the volume. A common wall-model used for high Reynolds number LES is defined as

\[
\sigma_{ij,s} = -u_*^2 \frac{u_{i,a}}{\langle |u_a| \rangle}
\] (3.32)

where \( u_* \) is the friction velocity and \( |u_{a}| \) the mean velocity magnitude at the first grid point above the wall (index \( a \)). For atmospheric flows, \( |u_{a}| \) and \( u_* \) are linked by the Monin-Obukhov (M-O) similarity theory (Monin and Obukhov 1954):

\[
\bar{u}_a = \frac{u_*}{\kappa} \left[ \frac{z_a}{z_0} + f_M \right]
\] (3.33)

where \( \kappa \) is the Karman constant, \( f_M \) the ABL stability correction function, \( z_0 \) the aerodynamic roughness length and \( z_a \) the distance between the surface and the first grid point. \( f_M \) must be prescribed a priori, depending on the stability of the ABL. The roughness length depends on the land usage (e.g. water, crops, forest, city). A classification can be found in Davenport (1960), Oke (1978), and Wieringa (1992). This
Another wall-model is the one proposed by Moeng (1984):

\[ \sigma_{ij,s} = \langle \sigma_{ij,s} \rangle \frac{\overline{u}_a \langle \overline{u}_{i,a} \rangle + \langle |\overline{u}_a| \rangle (\overline{u}_{i,a} - \langle u_{i,a} \rangle)}{\langle |\overline{u}_a| \rangle \langle u_{i,a} \rangle} \]  

(3.34)

This model and its modified versions was used by Mason and Callen (1986) and Albertson and Parlange (1999). Despite existing since several decades, there is still not a consensus within the LES community about the range of applications that suits the best a given model the best. Moreover, these models have been developed for flat wall bounded flow, while their behaviors in complex geometries (e.g. wall mounted cubes) is not known.

### 3.4 Reynolds Average Navier-Stokes

The Reynolds Average Navier Stokes (RANS) are based on the Reynolds average decomposition defined by Eq.2.4 and applied to the standard Navier-Stokes equations (see Eq.3.2). The pressure and the velocity appearing in the Navier-Stokes equations are replaced by their Reynolds decomposition

\[ p = \langle p \rangle + p' \]  

(3.35a)

\[ u = \langle u \rangle + u' \]  

(3.35b)

The new set of governing equations for RANS is defined as

\[ \frac{\partial \langle u_i \rangle}{\partial x_i} = 0 \]  

(3.36a)

\[ \frac{\partial \langle u_i \rangle}{\partial t} + \langle u_j \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} = - \frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial x_i} + \nu \frac{\partial^2 \langle u_i \rangle}{\partial x_i \partial x_j} - \frac{\partial \langle u_i' u_j' \rangle}{\partial x_j} \]  

(3.36b)

with Eq.3.36a the conservation of mass and Eq.3.36b the conservation of momentum. The last term of Eq.3.36b is the divergence of the Reynolds stress tensor, already presented in Section 2.1.3. It introduces six new unknowns in the system of equations. To close the system, \[ \langle u_i' u_j' \rangle \] is modeled by a RANS turbulence model. A tremendous number of models have been proposed in literature. The reader is
referred to Pope (2000) and Wilcox (2006) for more information about turbulence modelling for RANS. Similar averaging can be performed for each transport equation. For example the Reynolds-averaged equation for conservation of energy reads as:

\[
\frac{\partial \langle T \rangle}{\partial t} + \langle u_j \rangle \frac{\partial \langle T \rangle}{\partial x_j} = \alpha \frac{\partial^2 \langle T \rangle}{\partial x_j \partial x_j} - \frac{\partial \langle u'_i T' \rangle}{\partial x_j}
\] (3.37)

where \( \langle u'_i T' \rangle \) are the three turbulent heat fluxes. As they are new unknowns, the equation is closed with a RANS heat transfer model.

A transport equation for the Turbulent Kinetic Energy (TKE) \( k \) (Eq.2.10) can be derived from the RANS equation:

\[
\frac{\partial k}{\partial t} + \langle u_j \rangle \frac{\partial k}{\partial x_j} = \underbrace{- \langle u'_i u'_j \rangle \langle u_i \rangle / x_j}_{\text{production}} - \underbrace{\frac{\partial}{\partial x_j} \left[ \frac{1}{2} \langle u'_i u'_j \rangle + \frac{1}{\rho} \langle u'_i p' \rangle - \nu \frac{\partial k}{\partial x_j} \right]}_{\text{transport and diffusion}} - \underbrace{\nu \langle \frac{\partial u'_i \partial u'_j}{\partial x_j \partial x_j} \rangle}_{\text{pseudo-dissipation}}
\] (3.38)

The TKE production term

\[
P_k = - \langle u'_i u'_j \rangle \langle u_i \rangle / x_j
\] (3.39)

represents the transfer of energy from the mean flow to turbulence. The dissipation term is responsible for transforming the TKE of the smallest eddies into heat, via the viscosity \( \nu \).

### 3.5 One-way nesting for obstacles resolved LES

A nested LES-to-LES simulation is composed of an outer LES and an inner LES. The outer domain is dedicated to resolve the larger scales whereas the inner model solves the smaller scales. The outer domain encompasses the region that coincides with the inner domain, although at a lower resolution. With such an approach, the grid,
the timestep and even the physical model can be adapted to the scales resolved by each LES. In this thesis, Large scale LES (L-LES) is used to describe the outer domain. In the same manner, Small scale LES (S-LES) is used for the inner domain. The critical part in a nested LES-to-LES approach is the communication between the two models at runtime.

Figure 3.2a shows a sketch of a coarse-grained LES over an urbanized area. The domain covers a large horizontal extend. Due to the coarse grid, only relatively large turbulent structures are resolved and the eddies around the buildings are mainly under-resolved. Figure 3.2b shows the fined-grained LES embedded inside the L-LES. The turbulent fields of the L-LES are simply interpolated on the nested/coupled boundaries of the S-LES. This is a simple nesting procedure without blending. At the coupled inlet boundary, such interpolation is relatively straightforward as the coarse-grained eddies are simply advected with the flow. In the S-LES domain, new and finer turbulent structures develop due to the finer grid. Once at the outlet, the S-LES field is completely different as compared to the L-LES field. There is a mismatch between the advected S-LES structures and the imposed L-LES one, which leads to numerical instabilities. A simple solution would be to remove the nesting at the outlet, but the backward information from the building just after the outlet cannot be captured. Another solution is to place the outlet boundary in a region, where backward information is minimal. In a realistic case, like a urbanized area, such regions hardly exist. Figure 3.2c shows the same S-LES with a blending zone. In the vicinity of the nested boundaries, the fine-grained structures are transformed into the coarse grained eddies. With such blending, the feedback from the nearby structures is possible. It can also handle mixed inlet-outlet flow. This is a strong advantage for an obstacles-resolved LES.

The following sections present a one-way, downscale nesting procedure specifically designed for LES-to-LES simulations. An implicit blending procedure is added to the transport equations and a timestep interpolation is used to link the two LESs which are running at different timesteps.
Figure 3.2: Effect of the chaotic development of turbulent structures in a LES-to-LES nesting. The circles are schematic representations of turbulent eddies.
3.5.1 Model equations

The S-LES model solves a modified set of filtered Navier-Stokes equations, which include the blending between the coarse-grained $\bar{u}_i^L$ and fine-grained $\bar{u}_i^S$ field. This blending method is similar to the one proposed by Davies (1976) for RANS-Numerical Weather Prediction (NWP) nesting. The mass and momentum conservation equations become

$$\frac{\partial \bar{u}_i^S}{\partial x_i} = 0 \quad (3.40a)$$

$$\frac{\partial \bar{u}_i^S}{\partial t} + \bar{u}_j^S \frac{\partial \bar{u}_i^S}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p^S}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i^S}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}^S}{\partial x_j} + \frac{w}{\tau_r} (\bar{u}_i^L - \bar{u}_i^S) \quad (3.40b)$$

where the subscripts $^S$ and $^L$ represent the fields of the S-LES and the L-LES respectively, $w \in [0, 1]$ the blending factor and $\tau_r$ the relaxation time. The last right-hand side term represents the implementation of the blending. It is an implicit source term, which corrects the error between the computed field $\bar{u}_i^S$ and the target field $\bar{u}_i^L$. The higher the error, the stronger the correction. The implicit blending has several advantages on an explicit blending. An explicit blending procedure solves first the standard Navier-Stokes equations (Eq. 3.15) at each timestep, and then applies a blending procedure to the fine-grained $\bar{u}_i^S$ fields after being computed. From a physical point of view, the implicit procedure ensures that the blending is applied at solving time, without a time delay like in explicit procedures. Furthermore, the implicit method can handle complex inlet-outlet boundaries and avoid mismatches, as presented in Figure 3.2. An explicit method generally fails on this point, which leads to inconsistent results at best, or to a crash of solver most of the time.

The blending factor $w$ ensures a smooth transition from the non-blended region to the fully blended boundary. At the coupled boundaries, $w$ is equal to one and decreases to zero inside the domain as the distance with the coupled boundaries increases. $d_w$ is the characteristic distance from the coupled boundary to the region where $w = 0$ (see Figure 3.3).

The relaxation time $\tau_r$ controls the strength of the source term. A large $\tau_r$ weakens the coupling with the L-LES. The blending is less...
Figure 3.3: Top view example of a nesting between a L-LES and a S-LES. For clarity, only the inlet and the outlet of the inner domain are coupled to the outer one. The blending distance $d_w$ is defined for each of the coupled boundary.

efficient and therefore the S-LES fields are weakly affected. A small $\tau_r$ enhances the coupling. If it becomes too small, instabilities develop in the pressure field $\bar{p}^S$ near the coupled boundaries and the transition from the non-blended to the blended area is too sharp.

The blending procedure introduced in Eq.3.40b is applicable to any transport equation. For example, the filtered conservation of energy for the S-LES, with a blending term is defined as

$$\frac{\partial T^S}{\partial t} + \bar{u}_j^S \frac{\partial T^S}{\partial x_j} = \alpha \frac{\partial^2 T^S}{\partial x_j \partial x_j} - \frac{\partial u''_i T''^S}{\partial x_j} + \frac{\bar{u}T_L - T^S}{\tau_r}$$

(3.41)

3.5.2 Model time stepping and algorithm

The L-LES and the S-LES run with two different timesteps $\Delta t^L$ and $\Delta t^S$ respectively. Therefore for one coarse timestep, the S-LES computes several timesteps as shown in Figure 3.4. For the boundary coupling and the blending procedure, the turbulent fields from the L-LES are needed at each timestep of the S-LES. To obtain the "missing" coarse-grained fields, a linear interpolation is used between two consecutive $\Delta t^L$:

$$\bar{u}^L_{i+1/N_{\Delta t}} = \left(1 - \frac{i}{N_{\Delta t}}\right) \bar{u}^L_i + \frac{i}{N_{\Delta t}} \bar{u}^L_{i+1}$$

(3.42)

where $N_{\Delta t}$ is the nesting timestep ratio defined in Section 2.3.
Figure 3.4: Time step interpolation during a nested calculation. In this example, $\Delta t^S = (1/3)\Delta t^L$. The linear interpolation provides the "missing" $\bar{u}^L$ to $\bar{u}^S$.

The algorithm of the nesting procedure is described in Algorithm 1.

Algorithm 1 One-way, downscale nested LES-to-LES algorithm

1: for each time $t$ do
2:   compute $\bar{u}^L_t$ and $\bar{p}^L_t$ with Navier-Stokes (Eq.3.15)
3: for $k = 1, 2, ..., N_{\Delta t}$ do
4:   compute the sub-timestep $t_s = t - 1 + k/N_{\Delta t}$
5:   compute $\bar{u}^L_{t_s}$ with $\bar{u}^L_{t-1}$ and $\bar{u}^L_t$ (Eq.3.42)
6:   compute $\bar{u}^S_{t_s}$ and $\bar{p}^S_{t_s}$ with nested Navier-Stokes (Eq.3.40)
7: end for
8: end for

3.6 WALL-CLOCK TIME EVALUATION

Evaluation of the wall-clock time of a unsteady LES, or any unsteady Computational Fluid Dynamics (CFD), depends on a large number of parameters. A LES simulates the flow during the physical time $\Delta t_p$, which is discretized in a large number of timesteps $\Delta t$. At each timestep, the iterative solver does $n_s$ iterations on average. The wall-clock time $\Delta t_c$ spent to simulate the physical time is proportional to
the number of grid cells $N_c$ and inversely proportional to the timestep and the number of cpu $N_{cpu}$:

$$\Delta t_c = C_{ext} \frac{N_c}{N_{cpu} \Delta t}$$  \hspace{1cm} (3.43)

where $C_{ext}$ represents a coefficient depending on external parameters, such as the computer architecture, the solver type and the efficiency of the code (e.g: scalability). The wall-clock time for a nested LES-to-LES is simply the sum of each LES:

$$\Delta t_c^N = \Delta t_c^L + \Delta t_c^S$$  \hspace{1cm} (3.44)

where $\Delta t_c^N$ is the nested-LES wall-clock time.

The major interest of a nested LES-to-LES is its ability to simulate a wide range of scales in an acceptable wall-clock time compared to a standard LES. Assuming the same solver, same computer and same number of processors, the wall-clock ratio between a nested and a standard LES is defined as

$$\frac{\Delta t_c}{\Delta t_c^N} = N_c \left[ \frac{\Delta t_c^L}{\Delta t} + \frac{\Delta t_c^S}{\Delta t} \right]^{-1}$$  \hspace{1cm} (3.45)

This ratio only represents an estimation. The transfer of information in the nested simulation also requires time, although relatively small compared to the iterative solver, and the external parameters $C_{ext}$ can vary slightly between cases.

3.7 NUMERICAL SOLVER

This study uses OpenFOAM (Open source Field Operation And Manipulation) as CFD tool (Jasak 1996; Weller et al. 1998; OpenFOAM 2015). It is a collection of libraries, discretization methods and solvers to compute a wide range of problems in science and engineering. The code is open-source and written in C++ with an oriented-object paradigm.

The equations are discretized with the Finite Volume Method (FVM) on a collocated grid and can be applied on arbitrary topology and cell shape. Both segregated and implicit solvers are available in single or double precision. OpenFOAM comes with several linear solvers and multiple discretization schemes of first and second order in space and time.
The nesting procedure proposed in section 3.5 is specially designed to simulate the interaction between large atmospheric scales and small turbulent structures created by man-made structures in urbanized area. In this chapter, the nesting procedure is carefully validated against a reference simulation. The inner domain and the reference model share the same fine discretization in space and time, but the reference case has the same spatial extend as the outer model. The outer domain is coarser in space and in time.

The numerical models are detailed in Section 4.1. The effects of the blending procedure are shown in Section 4.2. The results of the numerical validation are presented in Sections 4.3 and 4.4. The former describes the turbulence statistics, whereas the latter shows the evolution of the spectra inside and outside the blending zone. In the discussion Section (Section 4.5), the effects of the blending parameter $\tau_r$ are explored in more detail, as well as the possibility of seeding of small scale eddies in the inner domain to trigger the development of fine turbulent scales. Finally, Section 4.6 presents the removal potential of a scalar from an urban area and how it is predicted by the nested simulation compared to the reference. Section 4.7 draws the main conclusions.

4.1 Numerical Model

The one-way, downscale nesting procedure described in Section 3.5 is designed to resolve turbulent flow problems which have two ranges of scales separated by one or more orders of magnitude. Resolving all those scales in a single Large Eddy Simulation (LES) domain would be computationally very expensive.

To validate the nesting procedure against a reference LES, the test case has to be chosen in such a way that the two ranges of scales are not too far apart, and all scales can therefore be resolved in the
reference model with acceptable computational requirements. For example, real buildings of 10 m height in an Atmospheric Boundary Layer (ABL) with its top 1000m Above Ground Level (AGL) hardly fulfill this requirement. Instead, in this study cubes embedded in a turbulent flow are used. All turbulent flows are composed of a wide range of scales, which are visible on a turbulent energy spectrum. The outer domain, with its coarse grid, can resolve only the largest scales of the spectrum. The inner domain can resolve much smaller eddies due to its fine grid. The reference LES has the same domain as the outer LES, but with a fine grid, similar to the grid of the inner LES.

4.1.1 Geometry and mesh

Figure 4.1 shows the two domains used for the numerical validation. The flow goes from left to right. The inner domain, also known as the Small scale LES (S-LES), overlays the outer domain, known as the Large scale LES (L-LES). The Reference LES (R-LES) domain has the same topology as the L-LES domain but with a mesh size equal to the S-LES. The cubes are placed in a staggered arrangement of six...
rows. With such configuration, the central line of cubes is completely immersed in the domain and far enough from the side boundaries. The R-LES and the L-LES domains are identical and cover all the rows plus an inlet fetch of 5\(h\) and outlet tail of 10\(h\). The vertical direction extents up to 6\(h\). The S-LES has the same vertical and spanwise extend as the outer domain. In the streamwise direction the inner LES covers only the two central rows, plus a half row at the inlet and outlet boundaries. The geometry is non-periodic in the streamwise direction, which is rather unusual for such a validation. This choice is motivated by the following points:

- This configuration is more similar to a real urban scenario, where dissipation and production of turbulence are neither isotropic, nor in equilibrium. The nesting procedure should be able to reproduce such effects, especially in the transition from the coarse-grained to fine-grained grid and vice versa.

- With cyclic boundary conditions, there is no control on the flow in the domain. A cyclic R-LES and L-LES would produce different flows, due to the difference of grid and timestep. Therefore the comparison between the reference and the inner domain would be impossible.

- As the domain is non-periodic in the streamwise direction, a turbulent inflow generator is used for the inlet boundary condition. This type of inflow generator will be required for the experimental validation (Chap. 5) and the realistic test case (Chap. 6). Hence, this geometry offers an interesting test bed.

Inflow generators require the statistics of the flow (mean and Reynolds stress) as well as the lengthscales. Statistics of boundary layers are easy to find in literature, but lengthscales are seldom presented as they are difficult to determine (i.e. large amount of data required or too noisy for integration). Instead of approximating lengthscale profiles, the numerical domain is scaled down to \(h = 0.05\) m to be able to use boundary layer data measured with time-resolved stereoscopic Particle Image Velocimetry (PIV) by Paterna (2015) in the wind tunnel of the laboratory.

Detailed views of the grids are shown in Figure 4.2. The grids are composed of cubic cells only, with sharp transitions between two
levels of refinement. Such a cell shape and refinement strategy avoid the propagation of numerical, hence non-physical, anisotropy in the turbulent fields. The reference and inner models have the same grid refinement. The fine-grained grids are 4 to 8 times finer than the coarse-grained grid of the outer domain. For all LESs, the grids are refined near the wall to keep the mean $\langle y^+ \rangle$ values between 1 and 4. Further details on the grids are given in Table 4.1. With such $y^+$, all the LESs can be considered as wall-resolved. This approach avoids the usage of a wall-model, which would add an extra parametrization in simulation. This extra source of uncertainty is not necessary for the validation of the nesting procedure. Nevertheless, this level of refinement at the wall is unfeasible in full-scale simulations.

![Detailed views of the grids used for each domain.](image)

<table>
<thead>
<tr>
<th></th>
<th>R-LES</th>
<th>L-LES</th>
<th>S-LES</th>
</tr>
</thead>
<tbody>
<tr>
<td>cell count</td>
<td>$9.2 \times 10^6$</td>
<td>$4.1 \times 10^6$</td>
<td>$4.1 \times 10^6$</td>
</tr>
<tr>
<td>mean cell size between the cubes</td>
<td>$h/32$</td>
<td>$h/4$</td>
<td>$h/32$</td>
</tr>
<tr>
<td>mean $y^+$ on the cubes</td>
<td>1 to 2</td>
<td>3 to 4</td>
<td>1 to 2</td>
</tr>
</tbody>
</table>

Table 4.1: Mesh specifications for all cases. All the cells of the grids are cubes, therefore the $y^+$ is the same in every directions.

The quality of the spatial discretization of a LES can not be evaluated by comparing the results of several grid refinement as is done in a
Reynolds Average Navier Stokes (RANS). Indeed, increasing the grid resolution will simply allows the LES model to resolve more turbulent structures. In fact, a LES becomes a Direct Numerical Simulation (DNS) if the grid is sufficiently refined and if the sub-grid scale (sgs) model becomes zero. Several methods exist to evaluate the grid quality of a LES. A first possibility is to compare the resolved Turbulent Kinetic Energy (TKE) with the total one. The higher the ratio, the better the resolution of the grid. A second method is to compute the spectrum and to compare it with the theoretical one (the $-5/3$ law). A well refined grid should have a wide range of resolved structures in the inertial sub-range. Another method is to compute the lengthscale from the two-points correlation and to find how many cell are used to resolve it. Finally, the two-point correlation function can be used to evaluate the grid quality by comparing the Taylor microscale. Davidson (2009) shows that two-point methods are the most accurate to evaluate the quality of a LES. According to his study, the other methods cannot provide accurate quantitative information of the grid quality, only a qualitative one.

The grid resolution of the LES presented in this chapter is evaluated with the ratio of the modeled TKE to the total one. This method has the great advantage to be easily computable at every location of the domain. The two-point correlation method cannot be applied in a complex geometry as it requires a certain distance in direction $r$ to be computed (see Eq. 2.15). The spectrum method can be computed at each location of the domain, but the comparison with the theoretical model can hardly be automated. Moreover, the two last methods are based on computationally expensive, fast-fourier transform and correlation, whereas the energy ratio method involves only statistical quantities. The TKE ratio $k_{res}$ is defined by the following relation:

$$k_{res} = \frac{k}{k + k_{sgs}} \quad (4.1)$$

According to Pope (2000), the mesh is sufficiently refined if $k_{res} > 0.8$. Davidson (2009) shows that a ratio of 0.8 might not be sufficient to evaluate the resolution; therefore, higher values should be selected (he does not specify a value). Figure 4.3 shows $k_{res}$ around the cubes. The TKE ratio is higher than 0.95 almost everywhere in the reference and the inner domain. The L-LES shows a lower TKE ratio than the
fine-grained models, especially between the cubes. Even if the ratio is still higher than 0.8, the effects of the under-resolved grid are clearly visible in the TKE and the Reynolds stresses. Therefore the R-LES and the S-LES can be considered as well-resolved, whereas the L-LES is under-resolved.

Figure 4.3: TKE ratio $k_{res}$ around the cubes. Cut plane at $y/h = 0$.

4.1.2 Boundary conditions

For the inlet boundary of the R-LES and L-LES, the turbulent inflow generator proposed by Kornev and Hassel (2007) is used. It generates a realistic turbulent flow using the mean profile, the Reynolds stress and the lengthscale $L_{I_1,1}$ as input. The profiles shown in Figure 4.4 are prescribed to the inflow generator to create the turbulent inflow. They are measured with PIV from the ETHZ/Empa wind tunnel by Paterna (2015). It is a boundary layer, which extends up to $z_i = z/h \approx 3.5$, with a mean freestream velocity of $\langle u_{f,s} \rangle = 2 \text{ m/s}$. With $\langle u_{f,s} \rangle$ as reference velocity, the block height $h$ as reference length and the
viscosity \( \nu u = 1.46 \cdot 10^{-5} \text{ m}^2/\text{s} \), the freestream Reynolds number is equal to \( Re_{fs} \approx 9000 \). The prescribed lengthscale is computed from the timescale by applying the Frozen turbulence hypothesis (Eq.2.19). The profile is forcefully set to 0 m above \( z/h = 3 \). It is done to avoid turbulence generation in the intermittent regime at the transition region between the turbulent boundary and the laminar freestream.

![Figure 4.4: Characteristics of the inlet profile used to feed the inflow generator. Measured by Paterna (2015).](image)

For the R-LES and the L-LES models, the normal velocity gradient is set to zero at the outlet boundary, the side boundaries are defined as cyclic and the top boundary is a symmetry plane. All the walls are modeled as smooth with a no-slip boundary condition. As the grid is sufficiently refined near the walls, with the \( x^+, y^+ \) and \( z^+ \) close to unity, the R-LES and L-LES are wall-resolved, therefore no wall-functions are used.

The S-LES has the same spanwise and vertical extend as the outer domain. Therefore the top and the side boundaries are not nested. Similarly to the L-LES, a cycle condition is applied to the side boundaries and the top is set as symmetric. The inlet and outlet boundaries are nested, or coupled, to the outer domain. For those boundaries, the coarse-grained velocity field is interpolated on the nested boundaries.
The implicit blending procedure described in Section 3.5 is applied to the S-LES. The blending distance is set to \( dw = h \) for both coupled boundaries and the relaxation time is set to \( \tau_r = 0.01 \text{s} \). The implications of those parameters is discussed in more detail in Section 4.5.1.

### 4.1.3 Turbulence model

The dynamic Smagorinsky-Lilly (Lilly 1992) sgs-model is used for all LESs. It is a dynamic algebraic model, which has proven very good behavior in various applications. Being an algebraic model, it also simplifies the nesting procedure: the turbulent quantities are only local values without history, therefore they don’t need to be nested.

### 4.1.4 Solver parameters

To keep the solution as stable as possible and to have a time discretization in balance with the spatial discretization, the Courant number \( Co \), defined as

\[
Co = \frac{u \Delta t}{\Delta x}
\]  

is kept below unity in all the computational domains. According to the S-LES and L-LES grid shown in Figure 4.2, the nested simulation has a mean grid nesting ratio of \( N_{\Delta x} \approx 3 \). With \( Co \leq 1 \), the timestep of each simulation is defined as

\[
\begin{align*}
\Delta t^L &= 12 \times 10^{-5} \text{s} \\
\Delta t^R &= \Delta t^S = 4 \times 10^{-5} \text{s}
\end{align*}
\]

Those values lead to timestep nesting ratio of \( N_{\Delta t} = 3 \).

With the timesteps (Eq. 4.3) and the grid data (Tab. 4.1), the wall-clock time ratio between the nested and the reference simulation can be estimated with Eq. 3.45. The computational time of the nested LES is about 1.7 times faster than the R-LES.

The second-order backward Euler scheme is used to discretize the time derivative and second-order centered schemes are used for all the spatial derivatives, except the advection term. It is discretized with a Gamma scheme (Jasak et al. 1999). It is a second-order scheme with
a Normalized Variable Diagram (NVD) limiter. A pure second-order scheme, which would be slightly less dissipative, cannot be used in this case, because it generates non-physical velocity oscillations at the cube edge. To avoid this problem, the Peclet number

\[ Pe = \frac{\bar{u}^M \Delta x^M}{\nu}, \] (4.4)

which is equivalent to the cell Reynolds number, should be smaller than 2 everywhere (see Ferziger and Peric 2002, chapter 3). This requirement is impossible to reach, therefore a scheme with a limiter is used.

OpenFOAM 2.3.0® (OpenFOAM 2015) is used for all the LES presented in this chapter. The pressure-velocity coupling is handled with the Pressure Implicit with Splitting of Operator (PISO) algorithm, with two pressure correction loops. The momentum equation is solved with a preconditioned bi-conjugate gradient (PBiCG) solver and the pressure equation uses a geometric-algebraic multi-grid (GAMG) solver. The implicit nesting procedure is implemented by the author in a new OpenFOAM solver. Its source code is available on github\(^1\), as well as examples (Vonlanthen and Immer 2015a).

### 4.2 Effects of the Blending Zone

Figures 4.5 and 4.6 show the resolved velocity magnitude \(|\bar{u}|\) at a randomly selected timestep. Both figures show only the field in a selected area around the cubes. The dashed lines represent the depth of the blending zone in the S-LES and the point-dashed lines the location of the coupled boundaries in the L-LES. The inflow generator creates relatively large structures from the inlet to \(z/h = 5\), as seen on the R-LES and L-LES contour plots. Once the flow reaches the first row of cubes, new turbulent structures are triggered by the bluff bodies. The turbulent structures generated between the cubes are strongly influenced by the grid refinement. The velocity fields of the fine-grained models have much smaller structures. Interesting observations can be drawn on the blending by carefully comparing the fields of the inner and outer domain. For example in Figure

\(^1\) [https://github.com/ETH-BuildingPhysics/ETH-OFTools-2.3.X](https://github.com/ETH-BuildingPhysics/ETH-OFTools-2.3.X)
Figure 4.5: Instantaneous velocity magnitude. The dashed lines represent the depth of the blending zone in the inner domain and the point-dashed lines the location of the coupled boundaries in the outer domain. Cut plane at \( y/h = 0 \).

In Figure 4.6, the feature "A" from the L-LES is almost identically reproduced inside the blending zone of the S-LES. After the blending area, new turbulent structures appear in the flow. It shows that the blending acts as expected, by enforcing the coarse-grained eddies in the inner domain and finer structures are created after the blending zone. Once the eddies are advected after the blending area, they further break up into finer structures due to the finer grid. This is the expected behavior of a turbulent flow. Similar observations can be seen at the coupled outlet as shown by the feature "B" in Figure 4.6. The fine structures of the S-LES are slowly transformed into coarse-grained eddies when they cross the outlet blending area.
Figure 4.6: Instantaneous velocity magnitude. The dashed lines represent the depth of the blending zone in the inner domain and the point-dashed lines the location of the coupled boundaries in the outer domain. Cut plane at $z/h = 0.5$.

4.3 STATISTICS

Figure 4.7 shows the mean velocity field $\langle u_1 \rangle$. The mean field is almost identical for all cases. The critical parts, such as flow detachment at the cube top, is well captured by the coarser grid of the L-LES as well as the finer grids of the R-LES and S-LES. The same is observed for the space between the cubes: the mean flow features are qualitatively and quantitatively very similar. The vertical profiles of $\langle u_1 \rangle$ shown in Figure 4.8, further confirm the excellent match between all the cases. The profiles are extracted along the lines L1 to L7 as defined in Figure 4.1. To better quantify the differences between the nested LES and the
Figure 4.7: Mean streamwise velocity. The dashed lines represent the depth of the blending zone in the inner domain and the point-dashed lines the location of the coupled boundaries in the outer domain. Cut plane at $y/h = 0$.

reference LES, the relative errors are added on the second $x$ axis. They are defined as

$$
\epsilon^L = \left| \frac{\langle u_1^R \rangle - \langle u_1^L \rangle}{\langle u_{fs} \rangle} \right| \quad (4.5a)
$$

$$
\epsilon^S = \left| \frac{\langle u_1^R \rangle - \langle u_1^S \rangle}{\langle u_{fs} \rangle} \right| \quad (4.5b)
$$

The S-LES error remains below 2% at almost every locations. It increases up to 4% at the roof top. The error of the L-LES remains around 4% with peaks up to 10% at the roof top.

The differences between the inner and the outer domains become more important once looking at the second order statistics. Figure 4.9 shows the resolved part of the TKE. Only the resolved part is shown to focus on the comparison of the transport quantities only ($\overline{u}$ in this
Figure 4.8: Mean velocity profile $\langle u_1 \rangle$ along the lines L1 to L7 with the relative error between the R-LES and the S-LES (Eq. 4.5). Markers displayed every $h/2$.

case) and their statistics. Indeed, the sgs-TKE is generated by the sgs model. As the model used in these LESs is purely algebraic, there is no transported fields. Therefore the physical quantities generated by the turbulence model are not transfered through the nested boundaries. The effect of the coarse-grained grid is clearly visible by comparing the L-LES and the R-LES. In the L-LES, the shear layer of TKE after the first cube is much smaller. The same lack of TKE is visible downstream.
of the two other cubes. At the location of the coupled inlet, the TKE level in the outer domain is at least twice smaller than in the reference. On the other hand, in the blending free part of the inner domain, the TKE field is qualitatively and quantitatively similar to the reference case. In the S-LES, the shear layer behind the second cube has a similar shape and intensity as in the reference case. In the blending regions,

![Graphs showing resolved TKE](image)

Figure 4.9: Resolved TKE. The dashed lines represent the depth of the blending zone in the inner domain and the point-dashed lines the location of the coupled boundaries in the outer domain. Cut plane at $y/h = 0$.

the energy levels match the ones in the outer domain, as expected. The effect of the blending is clearly visible on the vertical profiles of TKE shown in Figure 4.10. On line L1, where the blending factor $w$ is equal to one, the S-LES and L-LES profiles match well, while they differ a lot from the profile of the reference case. Further downstream, at the edge of the blending zone ($w = 0$, position L2), the S-LES starts to match the reference case. This indicates that the blending zone acts correctly as a buffer region between the two domains, and drives the coarse-grained solution slowly toward the fine-grained one. At
the beginning of the outlet blending, along line L6, the S-LES profile slightly overshoots the reference in the shear layer. At the outlet of the S-LES, where the blending is at its maximum intensity, the S-LES and the L-LES profiles have the same values, as expected.

Figure 4.10: Resolved TKE profiles along the lines L1 to L7. Markers displayed every h/2.
A major challenge in a LES with mesh refinement is the behavior of the sub-grid scale model through grid refinement. It raises the following questions:

- Which distance is needed for finer turbulent structures to develop in a coarse-to-fine mesh transition? Are the new fine structures realistic?

- How are the fine structures transformed after a fine-to-coarse mesh transition? Where does their TKE go?

In the case of a coarse-to-fine mesh refinement, the filter width decreases suddenly, thus smaller eddies can be resolved. Vanella et al. (2008) and Goodfriend et al. (2013) show that there is a discontinuity in the TKE level at a coarse-to-fine transition and a significant distance before the small scale eddies start to reconstruct. Both studies propose a smooth filter width transition to reduce the discontinuity, but a large filter further increases the distance of reconstruction of the small structures. In a fine-to-coarse transition, Vanella et al. (2008) describe an energy pileup effect visible in the TKE and the energy spectra: when the flow from a fine-grained mesh approaches a coarse-grained region of the mesh, its turbulent kinetic energy suddenly raises. He proposes a smooth transition of the filter width to reduce this effect.

The nesting procedures presented in this thesis can be seen as a coarse-to-fine grid refinement near the nested inlet boundary. Therefore the capabilities of the fine-grained S-LES to reconstruct small scale eddies from the coarse-grained L-LES fields are explored in more detail. The blending zone should act as a buffer region, where finer eddies build up slowly to reach the same energy level as in the reference simulation. Figure 4.11 shows the energy spectra $E_{11}$ in function of the frequency $f$. It is defined as the Fourier transform of the auto-correlation $R_{11}$, which is computed at the location P1 to P7.
Figure 4.11: Turbulent energy spectrum $E_1(f)$ at points P1 to P7 (P4 is not included). P1 and P7 are located at the nested inlet and outlet respectively. P2 and P6 are placed at the end of the blending zone, and the points P3 and P5 are in blending free area. The location of the points is given in Figure 4.1.

These points are located slightly above the top of the cubes (See Figure 4.1 for the exact location). On all six figures, the effect of the filter width is clearly visible between the R-LES and the L-LES. The spectrum of the reference simulation shows more energy at high frequency (small scale eddies). Moreover, the $-5/3$ slope is clearly visible on the spectra of the R-LES. At the location P1 the spectra of
the L-LES and the S-LES are the same, as expected. At location P2, the edge of the inlet blending area, the S-LES spectrum stands between the reference and the coarse-grained spectra. The small structures already exist in the flow, but the flow needs a longer distance to reconstruct the entire range of eddies allowed by the grid. Inside the blending free domain, at point P3 to P6, the energy spectra of the inner and the reference LES are in very good agreement.

The point P7 is located at the nested outlet. At this point, the S-LES still shows a large amount of energy at high frequency even though the blending is at its maximum intensity. This excess of energy occurs only at high frequencies, hence represents only a small fraction of the TKE. As shown on the last plot of Figure 4.10 (line L7), this small amount of TKE due to the small scales is not visible in the S-LES profile. As the nested simulation uses a one-way downscale nesting, there is no feedback to the outer domain. Therefore the energy pile up described by Vanella et al. (2008) does not exist.

4.5 Discussion

4.5.1 Effects and choice of the relaxation time

The purpose of the blending zone is to achieve a smooth transition between the coarse- and the fine-grained velocity fields. If the transition is too stiff, the fine-grained fields do not have enough distance to develop and the coarse fields are fully imposed in the blending zone. If the blending is too weak, the fine-grained fields remain mostly unchanged, which can be a problem at nested outlets.

The behavior of the blending procedure is controlled by the relaxation time \( \tau_r \). It appears in Eq.3.40b in the denominator of the last right-hand side term, which enforces the implicit blending in the momentum equation. The smaller the relaxation time, the stronger the blending. To understand how \( \tau_r \) influences the blending procedure, several nested simulations are performed. All the parameters of the L-LES and the S-LES remain unchanged except for the relaxation time, which varies in \([4 \cdot 10^{-5}, 1 \cdot 10^{-3}, 1 \cdot 10^{-2}, 1 \cdot 10^{-1}]\) s. The smallest value is equal to the solver timestep of the S-LES and the three other values are separated by one order of magnitude between each
other. Figure 4.12 shows the spectra at 6 locations for the reference LES, the outer LES and the 4 inner LES with varying relaxation time. For the point P1 at the nested inlet, all S-LES curves fall on the L-LES spectrum. The spectra at location P2 and P3 clearly show the effect of relaxation time. The S-LES with \( \tau_r = 1 \cdot 10^{-1} \) s reconstructs the missing small eddies the fastest. At the edge of the blending zone (P2), its spectrum has almost the same energy content as the reference spectrum. The S-LES with \( \tau_r = 4 \cdot 10^{-5} \) s requires a longer distance.
for the turbulence to reconstruct compared to the cases with larger $\tau_r$. With such a small relaxation time, almost no finer eddies appear in the blending zone, hence its spectrum is almost similar to the L-LES spectrum. At point P3 in the blending free zone, energy is still missing at high frequency.

At the edge of the outlet blending (location P6), almost all the S-LES spectra overlie the R-LES, except for S-LES with $\tau_r = 4 \cdot 10^{-5}$. Its small scale structures have already disappeared. At the nested outlet (point P7), all the S-LES with $\tau_r < 1 \cdot 10^{-2}$ are at the energy level of the L-LES. With $\tau_r = 1 \cdot 10^{-2}$, a small amount of energy still exists at the nested outlet. The case with $\tau_r = 1 \cdot 10^{-1}$ has developed non-physical instabilities at the outlet. The relaxation time is too large and the flow doesn’t match the nested boundary anymore.

The nested simulation used for the validation with the reference LES uses $\tau_r = 1 \cdot 10^{-2}$. From its results and the effects of $\tau_r$ on the blending, the following conclusion can be drawn:

- At the nested inlet, the blending is slightly too stiff. The spectrum of the inner domain does not completely overlap the spectrum of the reference domain. For example, $\tau_r = 1 \cdot 10^{-2}$s allows a faster reconstruction of the missing scales.

- At the nested outlet, the blending with the selected $\tau_r$ seams too weak: there is still energy at high frequency. $\tau_r = 1 \cdot 10^{-3}$s gives a better coupling at the nested outlet without affecting the flow at the edge of the blending zone, where $w = 0$.

Depending on the location of the blending area, the relaxation time can be optimized, depending if the boundary is clearly an inflow or an outflow. In case of a mixed boundary, a compromise has to be made on the relaxation time.

An important question is how to select the proper relaxation time. Figure 4.13 shows the integral timescale profiles along the lines L1, L2, L6 and L7. In the blending area of both coupled boundary, $\tau_r = 1 \cdot 10^{-2}$s is smaller than the integral timescale of the L-LES. As seen in Section 4.3, this is a good compromise and gives results for the S-LES, which match very well the reference LES. Nevertheless, it is difficult to know a priori the timescale in the L-LES, since it is highly case specific. To avoid the need for a priori specification of the
4.5 DISCUSSION

relaxation time, further work should focus on dynamically computing its value during runtime. Directly computing the timescale in the L-LES is possible but involves costly operations such as calculating and integrating the auto-correlation function. This also requires storing the time-resolved history of the flow, which can easily result in several terabytes of data to handle at runtime. A more practical alternative to this costly approach would be to use algebraic approximations of the timescale. Piomelli et al. (2015) proposes an approximation of the integral lengthscale $L_I$ as a function of the turbulent kinetic energy $k$ and the turbulent dissipation $\epsilon$. Both $k$ and $\epsilon$ can be extracted from the time resolved velocity field of the L-LES. They only involve averaging operations, which can be computed efficiently at runtime. Nevertheless, computing an accurate value of $\epsilon$ is considered as quite challenging because very long time series, hence long runtime, are needed. Another solution is to adapt a turbulent model as used in RANS simulations. Some of them solve a transport equation for the integral lengthscale. Such models, like the $k-L$ model proposed by Menter and Egorov (2005), can be modified to dynamically compute the length scale of the L-LES. The drawback of this method lays in the solving extra transport equations, which can impacts negatively the runtime. For both solutions, once $L_I$ is known, it can be converted

Figure 4.13: Integral timescale profile $T_{l1}$ along lines L1, L2, L6 and L7.
into the integral timescale by applying the Taylor hypothesis of frozen turbulence.

4.5.2 Seeding of synthetic small scale eddies

In this nested simulation presented above, the nesting ratio in space is between 3 and 4, depending on the location. With such ratio and geometry, the nesting procedure is able to reconstruct similar turbulent structures compared to the reference LES for a fraction of the computational cost. Further work should focus on the behavior of the nesting procedure in case of larger nesting ratio. Will the nested LES still be able to reproduce the missing small scale structures? How long should the reconstruction fetch be? Those issues are somehow similar to the issue of inflow generation for turbulent resolved simulations (LES or DNS). Mayor et al. (2002) present a RANS-to-LES nesting, where he uses a recycling method to provide fully turbulent fields to the nested LES. Fluctuations are extracted from a sampling plane downstream of the inlet. They are added to the mean fields of the RANS simulations, and used as turbulent inlet for the LES. Klein et al. (2003) and Kornev and Hassel (2007) proposed two different synthetic inflow generators (the second one is used in the LES presented in this Chapter). Such turbulence generators take a prescribed mean velocity and superimpose fluctuations according to the desired Reynolds stresses and correlation profiles. Despite being inflow boundary condition (hence 2D), both methods first generate a 3D turbulent field in a virtual volume. Then the turbulent field is extracted from a slice and interpolated on the boundary of the real volume.

All the methods cited above cannot be directly used in a LES-to-LES nesting because they all start from some sort of mean profiles. In such nesting, the outer LES already provides a turbulent field and it would be counterproductive to eliminate those existing fluctuations and then add synthetic ones. All the information from the large coherent structures from the L-LES would be lost. Instead synthetic turbulent generators can be modified to add only the missing small scales eddies to the $\overline{u_i^S}$ field located inside the blending zone.
4.6 TRANSPORT SCALAR RELEASE

The dispersion of a scalar in urbanized environment has become an important topic in research, urbanization planning, and emergency response. Pollutant dispersion is a typical example of scalar transported by the flow (Vardoulakis et al. 2003; Di Sabatino et al. 2012; Leitl and Meroney 1997). It can be chemically active or passive. Temperature and moisture represent other types of scalar transport, where their removal potential is of importance. They are in general active (buoyant effects on the flow, thermal plumes), but can be considered as passive under some circumstances (e.g. strong wind). Scalar transport can also be used as a tracer for air. Like smoke, the scalar shows "where" a certain portion of air is moving to.

This section evaluates the possibility to use a nesting procedure to reproduce a dispersion event. Therefore the results of the S-LES are compared to the R-LES. As the L-LES covers the same domain as the R-LES, but with a coarser grid, the influence of the grid refinement is evaluated by comparing the results of these two simulations.

4.6.1 Model setup and flushing procedure

In the geometry defined in Figure 4.1, two scalar release boxes are introduced between the cubes (see Figure 4.14a for the location of the boxes). The scalars $s_1$ and $s_2$ fill the boxes 1 and 2 respectively. The scalar has the same density and diffusivity as air. Therefore they can be seen as air tracers. Both boxes are active only a very short time $\Delta t_a = 0.00024s$. During this time, the scalar’s concentration is forcefully set to $C_{s_i} = 1$, with $s_i$ the scalar $s_1$ or $s_2$. $\Delta t_a$ compares as follows with the simulation timesteps:

$$\Delta t_a = 2\Delta t^L$$
$$\Delta t_a = 6\Delta t^S = 6\Delta t^R$$

After $\Delta t_a$, the concentration in the boxes can evolve freely and the scalars are flushed during an a priori unknown amount of time $\Delta t_f$. During $\Delta t_f$, the scalar flux $f_s$ through the three evaluation surfaces (Figure 4.14b) is computed at each timestep.
The turbulent flushing of a scalar is a stochastic and non-stationary process. This means that the standard time-average operation defined in Eq. 2.6 cannot be applied. Therefore statistics are computed with the ensemble-average, or ensemble-mean, defined by Eq. 2.5. The ensemble-average flux of the scalar \( s_i \) through the evaluation surfaces \( A \) is defined as

\[
\langle f_{s_i,A} \rangle_e = \left\langle \int_A \rho_{s_i} s_i \bar{u} \cdot n dA \right\rangle_e
\]

with \( \rho_{s_i} \) the density of \( s_i \), \( n \) the normal to surface \( A \) and \( \langle \cdot \rangle_e \) the ensemble-average operator. To apply this mean operator, \( N \) independent realizations of the flushing are needed. Unfortunately computing \( N \) simulations of the reference and the nested case would be extremely costly. To save computational time, each scalar is released several times during a single run of the reference LES and the nested LES. Figure 4.15 shows this procedure during the time line of a given LES model. At time \( t_1 \), the release box \( i \) is filled with the scalar \( s_i \). Then the flushing protocol defined by \( \Delta t_{a,i} \) and \( \Delta t_{f,1} \) is executed. All those events
represents the first realization of the scalar dispersion. A second realization starts at time \( t_2 \), following the same protocol. To be sure that the two realizations are independent, \( t_1 \) and \( t_2 \) must be separated by at least twice the timescale to fulfill the Nyquist criterion:

\[
t_2 - t_1 > 2T_I
\]  

(4.8)

with \( T_I \) the integral timescale (Eq.2.17). This procedure reduces the computational effort because the flow is computed only one time to achieve \( N \) realizations. Nevertheless, the run with the \( N \) scalars release is still much more time consuming than the flow simulation alone, as it has to solve \( N \) scalar transport equations.

For this study, 10 realizations of each scalar are computed on each domain. Time separation between two consecutive realizations is equal to \( t_{i+1} - t_i = 0.2s \). It is roughly 5 to 10 times bigger than the characteristic integral timescale as seen in Figure 4.13. As the geometry is symmetric along the axis \( x_1 \), the evaluation surfaces \( side1 \) and \( side2 \) can be combined into one. This manipulation doubles the number of realizations for the evaluation of the ensemble-average.
4.6.2 Results and discussion

Figure 4.16 shows the curves of the ensemble-mean flux through the top surface and one side surface (side1 and side2 are symmetric). The ventilation of the release box 1 occurs mainly through the top surface. The peak value of the flux is more than 2 times higher than the sum of the side fluxes. Form $t = 0$ s to $t = 0.1$ s the flux through the top boundary increases. After this point the flux decreases again until it reaches negligible values after $t = 0.6$ s. Figure 4.17 shows the flushing of $\langle s_1 \rangle_e$ at five selected times on a vertical cut planes at $y/h = 0$. As visible in the second row of plots at time $t = 0.05$ s, the scalar is diluted and spreads through the top evaluation surface. At time $t = 0.10$ s, (third row of plot), the area through which $S_1$ is spread increases, which explains the increasing flux from $t = 0$ s to $t = 0.1$ s. After the peak, the flux decreases exponentially.

The fluxes through side surfaces experience first a plateau from $t = 0$ s to $t = 0.10$ s, followed by an increase until $t = 0.15$ s (Figure 4.16). As visible in Figure 4.18, the scalar is pushed downstream the cube ahead of the release box from time $t = 0.0$ s to $t = 0.1$ s. Therefore
the fluxes through the side surface do not increase. After the side cubes, at time \( t = 0.15 \) s, the scalar starts to escape through the sides with a relatively high concentration (row 4 in Figure 4.18). Later on, \( S_1 \) is flushed through the downstream half of the side surfaces.

As visible in Figure 4.16, all the three LES models show the same flushing curves. By looking at the flow statistics (Figures 4.7 and 4.9), the mean flow is well captured by both L-LES and R-LES model, but the TKE levels are lower in the L-LES. Therefore the flushing from the release box 1 is mainly driven by the mean flow and less by turbulence exchange.
Figure 4.17: $\langle s_1 \rangle_e$ contours at different times extracted from a vertical cut plane at $y/h = 0$. 
Figure 4.18: \( \langle s_1 \rangle_e \) contours at different times extracted from an horizontal cut plane at \( z/h = 0.5 \).
Figure 4.19 shows the evolution with time of the ensemble-mean flux \( \langle f_{s2} \rangle_e \) through the top surface and one side surface. In this figure, the peak value of the fluxes occur just after the end of the release time for all evaluation surfaces. The flushing can be split in two parts. After the time \( t \approx 0.15 \) s, the rate of change of fluxes through is lower. All the three LES model predict the same flushing rate through the side surfaces. Through the top boundary, both fine-grained LES show similar flushing rates, whereas L-LES shows a slower decay. The driving physics for pollutant removal from the second release box has two sources: it is mainly driven by the mean flow through the side surface, whereas the contribution of turbulence is non-negligible for the flushing through the top boundary. The L-LES cannot capture the flushing rate very accurately due to its low TKE prediction (see the bottom plot of Figure 4.19).

Figure 4.20 shows horizontal cut planes at \( z/h = 0.5 \) of \( \langle s_z \rangle_e \) at five selected times. The subtle variations in flushing rate between the fine-grained LES and the coarse-grained LES is not visible in such plots.
4.6 Transient Scalar Release

Figure 4.20: $\langle s_2 \rangle_{e}$ contours at different times extracted from an horizontal cut plane at $z/h = 0.5$.

The accuracy of the simulation of pollutant dispersion strongly depends on the physics involved in the process. When the pollutant is mainly transport by the mean flow, coarse LES, also known as Very Large Eddy Simulation (VLES) can accurately predict the flushing. When the driving mechanism is turbulence, the computational model should be carefully selected. From this assessment, both L-LES and S-LES are able to compute similar flushing rate from the first release box. The L-LES is limited in the case of flushing from the second release box due to poor prediction of TKE in the L-LES.
This chapter proposes a numerical validation of the one-way, downscale LES-to-LES described in Section 3.5. The blending zones allow an arbitrary location of the nested boundaries by smoothing the transition between the outer and the inner domain. This is especially useful for atmospheric flows with resolved obstacles. The blending area avoids the problem of discontinuities in the nested fields at the coupled boundaries. It smooths the transition from the coarse-grained to the fine-grained LES. The blending method can be applied to any conservation equation, like for the temperature or turbulent quantities. For each equation, the blending intensity can be adapted via the relaxation time.

The nesting procedure is carefully compared to a reference simulation. The mean and higher order statistics profiles inside the blending free zone of the nested LES show very good agreement with the reference LES. In the blending zone, the fine-grained S-LES solution is smoothly transformed into the coarse-grained L-LES solution, which avoids mismatches at the nested boundaries. The S-LES is also able to generate the missing small scale turbulent structures and to match the energy spectrum of the reference LES. For the test case presented in this study, the nesting procedure reduces the computational time by 45% compared to the reference LES.

The quality of the blending is dependent on the relaxation time $\tau_r$. The smaller $\tau_r$, the better the coupling and it can then handle complex time-dependent inflow-outflow boundary conditions. But too small $\tau_r$ generate spurious pressure oscillation and the transition from the blended region to the blending-free regions is too sharp. For a large relaxation time, the coupling is weaker, but the small scale turbulent structures develop faster in the blending zone. The nested simulation presented in this chapter has the same relaxation time for the coupled inlet and outlet boundaries. It gives the best trade off between the coupling strength and the development of the small turbulent scales.

The optimal value for $\tau_r$ is in the range off the integral timescale. This information can be used to implement a dynamic relaxation time, calculated during runtime. For example in an improved nesting procedure, the lengthscale, hence the timescale, can be computed with algebraic approximations or transport equations.
The nested simulation used in this chapter has a nesting ratio in space and time equal to 3. With this ratio, the fine-grained LES is able to reconstruct the missing small turbulent scales efficiently. In case of a larger nesting ratio, the turbulent fields of the coarse-grained LES might not be sufficiently turbulent. Therefore seeding of the missing fluctuations could be an interesting option for the fine LES. Modification of existing synthetic turbulent generators can be used to solve such problem.
EXPERIMENT VALIDATION

In this Chapter, the nesting procedure is validated against wind tunnel measurements. The idea is to create an experiment in a multiscale configuration with two distinct ranges of scales.

In real atmospheric flows, the turbulent structures from the Atmospheric Boundary Layer (ABL) represent the large scales and the eddies from the buildings are the small scales. The experimental model is designed to imitate such a configuration. It generates a Convective Boundary Layer (CBL) over a finite area heated plate, with or without wall mounted cubes. For both configurations, five temperature differences $\Delta T = 0, 40, 60, 80$ and $100$ K between the heated surface and the incoming flow are used for the measurements. For all ten cases (two configurations with five $\Delta T$ each) the mean velocity, the turbulence statistics and the energy spectrum are measured with Particle Image Velocimetry (PIV). The mean temperature is measured with a custom made probe composed of an array of thermocouples. As this wind tunnel experiment is primarily designed for numerical validation, the flow upstream of the heated surface is measured in order to provide a full dataset for use in a numerical simulation.

Two numerical models are created to reproduce the flow fields of both configurations. A standard Large Eddy Simulation (LES) is used for the configuration without cubes and a nested-LES is used for the cases with wall mounted cubes. Both configurations are computed with three temperature differences: $\Delta T = 0, 60$ and $100$ K. The LESs solve the incompressible Navier-Stokes equations and Boussinesq approximation is used for the buoyancy. The validity of this approximation is discussed in the section 5.7.

5.1 BACKGROUND

The heat transfer from a horizontal heated surface has several important implications on the development of a boundary layer. When a
laminar neutral boundary layer impinges the leading edge of a heated surface, its thickness starts to increase. After a certain distance, horizontal vortices attached to the surface start to develop, forming rolls. Those rolls represent the first stage of turbulence and strongly enhance the heat transfer (Imura et al. 1978; Wang 1982). Further downstream, the thermal boundary layer becomes completely turbulent and chaotic with bubble-like structures rising above it (Kudo et al. 2003). The experiments proposed in literature to understand and quantify those effects are all performed on heated surfaces which are considered infinitely long, with negligible side effects and a smooth surface (Gilpin et al. 1978; Wang 1982; Chen et al. 1986).

The ABL is turbulent when it starts to interact with a warmer surface. The typical example is the transition from sea to land: the ABL above the cold sea is already turbulent before coming into contact with a warm landmass. Such conditions can be reproduced in special wind tunnels with heated floors and controllable velocity and temperature profiles at the inlet. Meroney and Melbourne (1992) proposed an overview of the existing facilities with such capabilities. Rey et al. (1979), Ogawa et al. (1981), and Ohya and Uchida (2004) have simulated the development of a CBL from a turbulent neutral boundary layer, capped or not by a thermal inversion layer. They are able to reproduce up to a certain extent the effect of buoyancy on the velocity and the Reynolds stress profile. The surface is assumed infinite, with minimal side effects. In general some roughness is included to match the reality.

The wind tunnel setup proposed in this chapter combines some aspects of both types of experimental studies presented above. First, a neutral turbulent boundary layer is developing over the wind tunnel inlet fetch intercepts a heated surface. From there, a turbulent CBL develops and grows until it reaches the wall mounted cubes, which are fully immersed in the turbulent boundary layer. The cubes generate their own small turbulent structures, which are influenced by the large buoyant ones of the CBL. This interaction between the two scales is used to validate the nesting procedure.
5.2 EXPERIMENTAL FACILITY

5.2.1 ETHZ/Empa Atmospheric Boundary Layer Wind Tunnel

Figure 5.1: Sketch of the ETHZ/Empa Boundary Layer Wind Tunnel.

The ETHZ/Empa Atmospheric Boundary Layer Wind Tunnel (Figure 5.1) is designed to measure the interaction between the lower part of an ABL and urban configurations (single building or cluster of buildings) or small terrain features. It is a closed-circuit design with the flow turning in counter-clockwise direction. It can also be operated in open-circuit to simulate pollutant dispersion for example. The open configuration is also used to flush the PIV particles after measurements.

The lower sketch of Figure 5.1 shows the different components of the wind tunnel. The fan and its engine are mounted in an aerodynamic pod, which is attached to the fan duct with rigid straighteners. To avoid vibrations, the fan duct is mounted on silencers and connected to the rest of the wind tunnel with flexible strips. The maximum power output of the engine is 110 kW. The fan speed can be adjusted between 25 rpm to 100 rpm, which allows a mean free-stream wind velocity in the test section ranging from 0.5 m/s to 25 m/s. A sliding
gate is placed after the first corner following the power block. The inlet and outlet ducts are located before and after the sliding gate. During the open-loop configuration, the gate is closed and the inlet and outlet ducts are opened. After the second corner, the diffuser, the settling chamber and the contraction reduce the turbulent intensity of the flow entering the ABL development section. Two meshed screens are mounted at the beginning and the middle of the diffuser. The settling chamber is equipped with several honeycomb and screen panels. The cell diameter of the honeycomb is 7 mm and the screen mesh is 5 mm. The honeycomb panels reduce the longitudinal turbulence by breaking down the turbulent structures and the screens act similarly on the crosswise turbulence. The contraction further reduces the turbulent intensity and provides a smooth transition between the settling chamber and the development section. The ABL development section is 7.8 m long and it is followed by the test section of 2.6 m long. Both are 1.9 m wide and the ceiling can be adjusted from 1.3 m to 1.6 m for streamwise pressure gradient control.

The test section is equipped with two traverse systems. The large traverse around the test section holds the PIV components, such as cameras and laser. It can move along all three directions. It is used mainly to move the camera and the laser at the desired position. The second traverse stands inside the test section. The position of the head is controlled by stepper motors with a step size of 0.01 mm. The head can be moved in all three directions inside a volume of 2.3 m × 1.6 m × 0.3 m, with an accuracy of 0.1/300 mm. Several probe types can be mounted on the head, such as Laser Doppler Anemometry (LDA), hot-wire probes and temperature probes. The traverse can be used for reference drives from an absolute coordinate system. This capability is particularly useful for model placement and laser sheet alignment.

5.2.2 Particle image velocimetry

The ETHZ/Empa boundary layer wind tunnel is equipped with a time-resolved, stereoscopic PIV system provided by LaVision. The images are recorded with two 12 bit CMOS-chip dual frame cameras. The maximum resolution is 2016 × 2106 pixels with a recording frequency of 640 Hz. With this resolution, 3155 double-frame images can be
stored on the 36 GB of memory installed in each camera. By reducing the resolution, the frequency can be increased up to 4502 Hz as well as the total number of images. Both cameras are equipped with a single axis Scheimpflug, which allows the alignment of the plane of focus with the laser sheet plane. The optics used are two 135 mm F2.0 Canon objectives. The laser sheet is produced by a diode-pumped Q-switched dual-cavity Nd:YLF laser with a wavelength of 527 nm. The maximum energy per pulse is 30 mJ at 1 kHz with a duration of 150 ns. The flow is seeded with 1 µm aerosol particles of Di-Ethyl-Hexyl-Sebacat (DEHS). It is assumed these particules have no influence on the flow momentum.

### 5.2.3 Air temperature probe

Vertical air temperature profiles are measured with a custom made array of thermocouples mounted on a fork-like structure, as shown in Figure 5.2. Due to its design, the probe is named the ThermoCouples Fork (TC-Fork).

The overall probe size is 250 mm × 40 mm × 63 mm. The structure is made of raw printed circuit board (PCB) where the copper layer is ground off. Such material allows rapid and precise prototyping with a PCB printer. As the PCB material is plastic, small modifications are easily feasible by hand. The spacers, located at the probe trailing edge, stabilize the structure and ensure a constant mechanical tension for each thermocouple.

The temperature is measured by 31 Type T (copper–constantan) thermocouples of 0.08 mm diameter. They are attached at the probe leading edge, in tension between the two arms of the fork (PCB supports). The lowest thermocouple (TC1) is placed 1 mm above the base of the TC-Fork. The distance between the thermocouples gradually stretches according to the following recessive law:

\[
dTC_{i+1} = dTC_1 + dTC_i + 0.25i
\]

where \(dTC_i\) is the distance from the TC-Fork base to the thermocouple \(TC_i\) and \(i \in [1, 30]\). Therefore the second thermocouple is placed 1.25 mm above the first one and the third one 1.50 mm above the second one. The distance between the second to last and the last
Figure 5.2: The ThermoCouples Fork (TC-Fork) used for temperature measurements. (a) the CAD model and (b) the actual probe mounted in the wind tunnel model. In the CAD view, the thermocouple wires of 0.08 mm diameter are magnified by a factor 10 to make them visible. The black spheres on the thermocouples indicate the location of the thermocouple junctions, hence where the temperature is measured. In reality the junction has the same diameter of the wire.

thermocouple is equal to 8.5 mm. The total measurement height is 147.25 mm. An extra thermocouple (ground TC in Figure 5.2b) is used as reference measurement. In general, it is used to measure the temperature of the heating device (the ground in this case).

The wires of the thermocouples (TC-wires in Figure 5.2b) run on the external side of each PCB supports, until they arrive at the channel switching board. The voltage of each thermocouple is sent sequentially from the switch board to the compensation box equipped with a platinum wire PT100, which measures the reference absolute temperature.
5.3 Model Setup

The compensation box converts the voltage difference $\Delta V$ between the copper and constantan wires into an absolute temperature. After calibration, the error on the absolute air temperature measured by the TC-Fork is $\pm0.2\,\text{K}$. With this acquisition chain, the maximum measurement frequency is $0.1\,\text{Hz}$.

5.3 Model Setup

A sketch of the experimental setup is displayed in Figure 5.3. The setup is mounted on the floor of the wind tunnel and has a total size of $448\,\text{cm} \times 178\,\text{cm}$ with a thickness of $6\,\text{cm}$. The heated surface is composed of 6 heated plates of $60\,\text{cm} \times 20\,\text{cm}$ and 6 others of $60\,\text{cm} \times 10\,\text{cm}$. The last 6 plates are attached two by two to form $60\,\text{cm} \times 20\,\text{cm}$ plates. The surface of each heated plate is made of a $5\,\text{mm}$ aluminum sheet. An electro-resistive heating mat is glued on the bottom of each aluminum plate. It can deliver a maximal power output of $1680\,\text{W}$. With this power, temperatures of more than $140\,\text{°C}$ can be easily reached. As the aluminum is an excellent thermal conductor, the temperature of the plate’s surface remains uniform throughout the experiment. The target temperature is reached using a PID controller.
The aluminum plate and the heating mat lay on a 5 cm insulated sheet of incombustible mineral wool, encapsulated in a support to ensure the stability and the flatness of the setup. A fairing made of structural foam is placed around the heated surface to smoothen the transition from the wind tunnel floor to the model. The side insulation, made of mineral wool, avoids heat leakage to the fairing. The inlet mirror (Figure 5.3) is used to reduce the scattering of the laser sheet during the PIV measurement of the inlet profile. The array of bluff bodies is composed of three cubes with a height of $h = 5\text{ cm}$. They are not actively heated and warm up only by conduction with the plates. They are made of bulk steel with an electro polished surface finishing to reduce the laser scattering (Paterna et al. 2013). Aluminum would have been a better choice regarding thermal conductivity, but the scattering reduction is the prime concern in this case. The last cube of the array (the downstream one) is placed 32.5 cm from the rear edge of the heated surface. The cubes are mounted on the aluminum plate in dry contact (no thermal paste used). They are neither attached nor screwed. With this setup, the experiment can be easily switched from the wall mounted cube setup to the flat wall setup.

The camera is mounted spanwise of the mean flow direction (see Figures 5.4). The setup is a planar (2D), 2 components PIV, also known as 2D2C PIV. Therefore only the $u_1$ and $u_3$ components are measured. The field of view is $\approx 20\text{ cm} \times 20\text{ cm}$ ($4h \times 4h$). Its leading edge is aligned with the downstream face of the second cube (Figure 5.5). In this configuration, the last cube is completely visible by the camera and the velocity field can be measured up to $2h$ downstream of the last cube and $\approx 4h$ in the vertical direction.
Figure 5.5: Side view of the experimental setup, with the PIV fields of view and the locations of the sampling line L1 and point probe P1 to P4. For the setup without cubes, the sampling location and the field of view are similar.

In order to measure the velocity as close as possible to the heated surface, the camera and its Scheimpflug are mounted specifically to have the bottom part of the cone of view aligned with the ground (Figure 5.4). With this configuration the noise due to the laser scattering from the ground is strongly reduced as the surface of the model is never visible in the camera. The drawback of such mounting is the impossibility to use the stereoscopic capability of the PIV system. Indeed, because the Scheimpflug is already in use to align the cone of view with the ground, therefore it cannot be used to sharpen the whole image in a stereoscopic setup. The only way to handle both would be to use a double axis Scheimpflug (Walker 2001). For the setup without cubes, the streamwise dimension of the camera’s field of view is reduced to $h \times 4h$ (see camera narrow FOV in Figure 5.5). With such a narrow field of view, the camera can record more images and with higher frequencies if needed. This provides a higher number of independent samples for the statistics, and a longer time-series of time-resolved images at high frequency for the spectral analysis.

The inflow data is measured with PIV above the mirror, as seen in Figure 5.3. The camera is mounted as shown in Figure 5.4. As for the measurement without cubes, the camera field of view is reduced to $h \times 4h$. 
Figure 5.6 shows the mounting of the temperature probes on the heated surface. The thermocouple array of the TC-Fork is aligned with the sampling line L1 (Figure 5.5), the same line used to extract PIV profiles. The TC-Fork is designed to be mounted on the inner

traverse head. Unfortunately, with this montage the fork vibrates due to the turbulent flow. The possible sources of vibrations are listed below:

- Due to its lightweight construction, the stiffness of the TC-Fork is too low. It can be improved by using stiffer materials for the structure, such as high density plastic or aluminum.

- The BCP supports of the fork are full plates. Therefore a slight misalignment with the flow generates high drag and vibrations due to turbulence. A hollow design associated with a stiffer material would solve this problem.

Figure 5.6: Side view of the experimental setup, with the position of the TC-Fork. The thermocouple array is aligned with the PIV sampling line L1 (see Figure 5.5).
• The vertical arm of traverse can slightly rotate around the transversal beam. If the arm is fully extended, like when a probe is close to the ground, vibrations can be amplified.

To avoid vibration, the TC-Fork simply stays on the heated plate with a downstream stand attached to it. The ground temperature is measured with the extra sensor of the TC-Fork. Figure 5.2b shows the fork in place behind the last cube, as well as the ground thermocouple.

The surface temperature of the second and third cubes is measured with four extra thermocouples, two per cube. The sensors $TC_{ia}$ are attached to the side faces and the $TC_{ib}$ sensors to the top face. See Figure 5.6 for the detailed positions.

5.4 MEASUREMENT PROTOCOL

The model has two configurations: with or without cubes mounted on the heated surface. For each configuration, five different cases are measured with a temperature difference $\Delta T$ between the plate and the air inflow from 0 K to 100 K. For each case, the air flow is measured with the PIV system. The air temperature profiles are measured with the TC-Fork. As the temperature probe is right in the PIV field of view, the TC-Fork is not mounted during the PIV recording. The temperature is measured later. For all measurements, the fan speed is set to 40 rpm, which gives a mean freestream velocity at the inflow of $\langle u \rangle_{fs} = 1.1$ m/s. The inflow temperature $T_{in}$ is equal to 23.4°C. The heating of the air inside the wind tunnel is limited to 0.5°C during a day of measurement. It remains low due to the large quantity of air involved in the wind tunnel and also the high thermal mass of the tunnel. The boundary layer thickness at the inflow (above the mirror) is equal to $L_{BL} = 0.125$ m. The height is determined when the boundary layer velocity reaches 99% of the freestream wind speed. Where $\langle u \rangle_{fs}$ is the reference velocity, $L_{BL}$ the reference length and $\nu = 1.46 \cdot 10^{-5}$ m$^2$/s the air viscosity, the Reynolds number of the measurements is $\approx 9400$. According to the literature, this is high enough for Reynolds independence in the CBL (Uehara et al. 2000). The bulk Richardson number for each case is shown in Table 5.1. $L_{BL}$ and $T_{in}$ are used as references to compute $Ri_b$. According to the definition of the Richardson number (see Section 2.2.1), in those
cases the Turbulent Kinetic Energy (TKE) generated by the buoyancy represents \( \approx 25\% \) of the TKE produced by the friction with the wall. Therefore they represent mixed-convection cases. At full scale, those numbers represent a relatively weak CBL.

<table>
<thead>
<tr>
<th>( \Delta T [\text{K}] )</th>
<th>( Ri_b )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.00</td>
</tr>
<tr>
<td>40</td>
<td>-0.14</td>
</tr>
<tr>
<td>60</td>
<td>-0.20</td>
</tr>
<tr>
<td>80</td>
<td>-0.27</td>
</tr>
<tr>
<td>100</td>
<td>-0.33</td>
</tr>
</tbody>
</table>

Table 5.1: Bulk Richardson number \( Ri_b \) according to the temperature difference between the heated surface and the inflow air.

Two types of PIV measurements are performed: the low frequency, time-average recording and the high frequency, time-resolved recording. The former is used to compute statistics and two-point correlations and the latter for spectral analysis and auto-correlations. The PIV parameters for each configuration and for the inflow measurement are presented in Table 5.2. The configuration without cubes and the inflow measurement are recorded with a cropped field of view (504 \( \times \) 2016 pixels) to increase the number of images, whereas the configuration with cubes are measured with a full field of view (2016 \( \times \) 2016 pixels).

<table>
<thead>
<tr>
<th>PIV parameters</th>
<th>configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>inflow</td>
</tr>
<tr>
<td>FOV size [mm]</td>
<td>50 ( \times ) 200</td>
</tr>
<tr>
<td>FOV size [pixel]</td>
<td>504 ( \times ) 2016</td>
</tr>
<tr>
<td>TR Img frequency [Hz]</td>
<td>500</td>
</tr>
<tr>
<td>AV Img frequency [Hz]</td>
<td>5</td>
</tr>
<tr>
<td>Nb of images</td>
<td>12 620</td>
</tr>
<tr>
<td>window size [pixel]</td>
<td>32 ( \times ) 32</td>
</tr>
</tbody>
</table>

Table 5.2: Parameters for Time-Resolved (TR) and Time-Average (TA) PIV.
5.5 Wind Tunnel Results

The final interrogation window size is equal to $32 \times 32$ pixels for the configuration without cube and the inflow measurements, whereas the interrogation window is reduced to $24 \times 24$ pixels for the configuration with cubes. This modification increases the PIV resolution, which will help to capture the expected small turbulent structures in the cubes wake. It also helps to measure sharp velocity gradients, which are generally present in the shear layers generated by the cubes. On the other hand, a smaller interrogation window decreases the peak-ratios (signal to noise) of the PIV correlations for the velocity vector search. In this set of measurements, the peak-ratio remains at a very good level for both window sizes. To put those numbers in perspective, the $32 \times 32$ interrogation window gives a resolution of $\approx 3.2 \times 3.2$ mm, whereas the $24 \times 24$ window goes down to $2.4 \times 2.4$ mm. For all the configurations, the window overlap is $50\%$.

5.5 Wind Tunnel Results

5.5.1 Flow statistics

Figure 5.7 shows the mean streamwise velocity $\langle u_1 \rangle$, the 2D Turbulent Kinetic Energy (TKE) $k_{2D}$ and the mean temperature difference $\Delta \langle T \rangle$ for the configuration without cubes. The mean temperature difference is defined as:

$$\Delta \langle T \rangle = \langle T \rangle - \langle T_w \rangle$$

where $\langle T_w \rangle = T_w$ is the heated plate temperature. As the measurements are done with a planar, 2 component PIV, the out-of-plane velocity component is not available, and set to zero. Therefore the formula of the TKE $k$ reduces to:

$$k_{2D} = \frac{1}{2} \langle u_1' u_1' + u_2' u_2' \rangle$$

As visible in Figure 5.7, the CBL grows thicker with increasing $\Delta T$. The heated cases have a deficit of speed from $z/h = 0.25$ up to $z/h = 3$ (Figure 5.7a), while turbulent kinetic energy is still present above $h/z = 2$. The peak value of $k_{2D}$ is located very close to the ground at $z/h = 0.1$ for all cases. Above the peaks, the heated cases have two to four times more $k_{2D}$ than the neutral case. Whereas the four heated cases are evenly distributed from $\Delta T = 40$ K to $\Delta T = 100$ K, $k_{2D}$ does
not follow the same trend. The cases $\Delta T = 40 \, \text{K}$ and $\Delta T = 60 \, \text{K}$ are grouped together, as well as the two warmer cases (Figure 5.7b). A similar clustering is found in the mean velocity shown on Figure 5.7a, especially from $z/h = 0.1$ to $z/h = 1$. The possible sources of this clustering effect are given later in the text. The mean difference of temperature is displayed in Figure 5.7c. Immediately above the ground, the gradient of temperature is very high up to $z/h = 0.1$. After this point, the temperature difference decreases slowly to $\Delta T = 0 \, \text{K}$ above $z/h = 3$.

The three available components of the Reynolds stress are shown in Figure 5.8. $\langle u'_1 u'_1 \rangle$ and $\langle u'_3 u'_3 \rangle$ are the two components contributing to $k_{2D}$ (Figures 5.8a and 5.8b). Below $z/h = 0.2$, $\langle u'_1 u'_1 \rangle$ is the main contributor to $k_{2D}$, whereas above $z/h = 0.2$ both components have a similar contribution. The vertical stresses of the heated cases are two to three time higher compared to the neutral case. The shear stresses are shown in Figure 5.8c. The shear stresses of the heated cases show a similar grouping as the one observed in Figure 5.7. The streamwise stresses also show the same type of clustering below $z/h = 2$, but
5.5 Wind Tunnel Results

Figure 5.8: Measurement without cubes: Reynolds stresses along line L1.

not the vertical stresses \( \langle u'_3 u'_3 \rangle \). They are evenly distributed with the increase of \( \Delta T \).

The clustering effect on this particular geometry (a finite area heated plate) can be explained by a transition of flow regime between \( \Delta T = 60 \text{ K} \) and \( \Delta T = 80 \text{ K} \). Such flow transition is known to exist in the development of a laminar CBL (see Kudo et al. 2003, and the explanations given in Section 5.7). The measurements presented in this chapter deal with the development of a turbulent CBL, but a similar type of flow transition might also exist. The clustering effect might be also due to the finite size of the heated surface. Above a given \( \Delta T \), the edge effects can become important. Measurement of the off-plane velocity at the centerline and at the edges of the heated surface can help to answer this question. The vertical turbulent temperature flux \( \langle u'_3 T' \rangle \) can also lead to interesting insights. This term appears in the Reynolds-averaged energy equation (Eq. 3.37) and it is responsible for the vertical transport of energy. Both the velocity and the temperature fluctuations are needed at the same time to compute this term. A hot-and-cold wire probe would fulfill this requirement.
Unfortunately, such equipment was not available when the experiment was conducted.

The mean streamwise velocity $\langle u_1 \rangle$ and the 2D TKE $k_{2D}$ for the configuration with cubes are displayed in Figure 5.9. Each row of plots represents the data for a given $\Delta T$ case. The main influence of the heating on the mean streamwise velocity is located downstream of the last cube. The area of the recirculation zone decreases until the case $\Delta T = 60$ K, and then stays relatively constant at higher $\Delta T$. The evolution of $k_{2D}$, with the increase of $\Delta T$, is presented in the second row of plots of Figure 5.9. In the neutral case, $k_{2D}$ shows high levels in the shear layer generated by the third cube and in the area where the shear layer of the second cube interacts with the upstream face of the last cube. At $\Delta T = 40$ K, those two zones of high $k_{2D}$ remain, but with lower intensity. As the temperature difference increases, the peak values of the two zones increase steadily, as well as their area. This decrease of intensity is unexpected. It can be explained by the velocity profile above the cubes. As shown in the first column of Figure 5.9, the boundary layer of the case $\Delta T = 40$ K is slightly thicker than in the other cases. Therefore the velocity at the cubes top in this case is about 5% to 7% lower compared to the other cases. This can explain the reduction of the turbulent kinetic energy and the Reynolds stress. Nevertheless, the reason why the boundary layer at $\Delta T = 40$ K is thicker is not clearly identified.

Figure 5.10 shows two components of the Reynolds stress tensor, the horizontal turbulent flux $\langle u'_1 u'_1 \rangle$ and the vertical one $\langle u'_3 u'_3 \rangle$. At $\Delta T = 0$ K, the horizontal turbulent flux starts to develop downstream of the upper edge of the last cube and then quickly extends. The shear layer from the second cube splits at the upstream edge of the third cube. A minor part is transported along the roof of the cube, whereas the majority is convected downward the upstream face of the third cube. At $\Delta T = 40$ K, the patterns of high $\langle u'_1 u'_1 \rangle$ are similar, but decrease in intensity. With increasing $\Delta T$, the horizontal turbulent flux strengthens in both shear layers and spreads in the vertical direction. The vertical turbulent flux in the neutral case reaches its peak value in the shear layer downstream of the last cube. Unlike $k_{2D}$ and $\langle u'_1 u'_1 \rangle$, there is almost no vertical turbulent fluxes in the shear layer from the second cube, but only a rather wide patch of high $\langle u'_3 u'_3 \rangle$ along the upstream face of the third cube. The intensity of the vertical turbulent
flux decreases at $\Delta T = 40$ K. As the temperature difference increases, the intensity gets higher and the patterns size extends, especially in the vertical direction. The effect of an increase of $\Delta T$ is particularly visible near the upstream face of the last cube. The intensity of the vertical turbulent flux increases faster than in the shear layer downstream. At $\Delta T = 80$ K and higher, the peak value of the $\langle u_3' u_3' \rangle$ is even located between the two last cubes.
Figure 5.9: Measurements with cubes: contours of the mean streamwise velocity $\langle u_1 \rangle$ and 2D TKE $k_{2D}$. Field of view on the last cube only.
Figure 5.10: Measurements with cubes: contours of the Reynolds stress components $\langle u_1'u_1' \rangle$ and $\langle u_3'u_3' \rangle$. Field of view on the last cube only.
The temperature data measured by the TC-Fork on the wall mounted cube configuration are given in Figure 5.11. The left plot (Figure 5.11a) shows the mean temperature difference $\Delta \langle T \rangle$ profiles between the air and the heated plate for the four CBL cases. As in the configuration without cubes, the profiles have a very sharp gradient near the ground. In the wake of the last cube, more heat remains entrapped in the recirculation zone, which leads to an increases of the temperatures from $z/h = 0$ to $z/h = 1$, compared to the configuration without cubes (Figure 5.7c).

The right plot (Figure 5.11b) gives the temperature difference between the cube thermocouples and the heated surface for each CBL case. The cubes are always at least 1 K colder than the heated surface. The temperature difference between the top and the side thermocouple of the second cube is about 0.05 K in all cases, whereas this difference is around 0.03 K for the third cube. Those differences are due to aerodynamic cooling. The top faces are the coldest because of
the higher convective heat transfer due to high wind speeds, whereas the side faces are slightly warmer. The side boundary are immersed in the low speed wake generated by the cubes, therefore the convection is reduced.

5.5.2 Spectra and turbulent scales

The spectra presented in this section are computed in function of the wavenumber $\kappa$. Therefore a given spectrum provides information about the amount of turbulent kinetic energy according to the size of the eddies. All the spectra are computed at the location P1 to P4, as shown in Figure 5.5.

The spectra for the configuration without cubes are shown in Figure 5.12. P1 is the lowest point and P4 the highest. All the turbulent spectra have a horizontal tail at high wavenumber, which is the noise

![Graphs showing spectra for different $\Delta T$ at locations P1 to P4.](image)

Figure 5.12: Spectra for the configuration without cubes for different $\Delta T$. The spectra are computed at location P1 to P4.
Figure 5.13: Spectra for the configuration with cubes, for different $\Delta T$. The spectra are computed at location P1 to P4.

from the PIV system. Before the tail, all the spectra follow the $-5/3$ law. For each location, the cases with ground heating overlap and show no significant differences. At location P1, the spectra of the neutral case and the heated one are similar. A bit higher, at location P2, the neutral case loses energy in the small scales (high wavenumber). At higher locations (P3 and P4), the loss of energy expands to all the wavenumber numbers. This effect is coherent with the TKE profiles shown in Figure 5.7. The neutral case has a lower TKE than the heated cases. The difference between the heated cases seen in the $k$ profile are not visible in the spectra. They are likely due to large coherent structures (hence low frequency), which are difficult to capture in the spectrum of a finite time-series.

Figure 5.13 shows the spectra from the configuration with cubes, at the locations P1 to P4. Similar observations can be made on those spectra like the one computed for the configuration without cubes.
The heated cases, as well as the neutral case are clustered together for locations P1 to P3. At location P4, the large scales (small $\kappa$) of the neutral cases has a lower energy.

The spectra from the configuration with and without cubes are compared in Figure 5.14. For clarity, only the cases $\Delta T = 0 \text{K}$ and $\Delta T = 60 \text{K}$ are shown for each configuration. At location P1, the small scale turbulent structures are more energetic than their counterpart in the configuration without cubes. Those small energetic eddies are primarily triggered by the upstream cubes. At location P2, at the cube height, the effects of the shear layer are clearly visible. The configuration with cubes has more energy at all wavenumber. At the higher locations (points P3 and P4), all the spectra come closer to each other as the influence of the cubes becomes weaker. At point
experiment validation

P4 the two spectra from the heated cases almost match, whereas the curves from the neutral cases matches only at a low wavenumber. Interestingly, this shows that the influence of the cubes seems to extend higher into the neutral boundary layer. In the CBL, the effects of the cubes almost disappears at location P4: the green and orange curves almost overlap, because the influence of the cubes slowly vanishes.

5.6 Nested Simulations

The LES models presented in this section are designed to reproduce the experimental conditions described in Section 5.3 and 5.4. The configuration without cubes is modeled by a standard LES model (no nesting used) and the configuration with cubes is reproduced by a nested LES model, which uses the nested procedure described in Section 3.5 and is validated against a reference simulation in Chapter 3. The nested LES is composed of two domains: the outer, or coarse-grained domain and the inner, or fine-grained domain. As in the previous chapter, the LES solution of the outer domain is known as the Large scale LES (L-LES) and the inner domain solution is the Small scale LES (S-LES). For simplicity, the LES without cubes is named Flat plate LES (F-LES).

For each model, the results are computed for three $\Delta T$. The neutral case with $\Delta T = 0$ K, and two heated cases with $\Delta T = 60$ K and $\Delta T = 100$ K. In the following sections, all six LES (two configurations with three $\Delta T$) are compared with their experimental counterparts.

5.6.1 Domains and grids

Figure 5.15 shows the computational domain of the L-LES and the F-LES. The latter has the same domain, but without the cubes mounted on the heated surface. $h$ is the height of the cubes. Compared to the wind tunnel setup, the LES domain covers the entire heated surface ($180 \text{ cm} \times 60 \text{ cm}$) plus an inlet and outlet fetch. The inlet is placed $6h$ ahead of the leading edge of the heated plates, at the exact location where the inflow profiles have been measured with PIV (see the label mirror in Figure 5.15a). The outlet is located $4h$ after the heated surface. The side boundaries are placed $6h$ apart from
the centerline. The LES domain covers only the heated surface in the spanwise direction. Several F-LES with a domain three times wider, hence as wide as the wind tunnel, have been tested. They did not show any significant difference when compared to the standard width F-LES. Therefore, the smaller domain presented here is selected, as it strongly reduces the number of grid cells. The domain extends up to $16h$ in the vertical direction.

The S-LES domain of the nested simulation is presented in Figure 5.16. It covers a distance of $8h$ in the streamwise direction, from downstream of the first cube at $32.5h$, to $39.5h$. Despite being much shorter than the L-LES domain, it is sufficient to cover the PIV measurement region (see Figure 5.15b and 5.16a). The domain extends up to $6h$ in the vertical direction and $6h$ in the spanwise direction. All the boundaries, except the walls, are nested to the outer domain with a blending distance $d_w = h$. 

Figure 5.15: Horizontal (a) and vertical cut of the L-LES domain. The F-LES domain is the same, but without cubes. $h$ is the cube height. For comparison, the PIV field of view is represented by the dashed red square.
Figure 5.16: Vertical (a) and horizontal cut (b) of the S-LES domain. \( h \) is the cube height.

In all domains, the line L1 is used for profile sampling. As the sampling line of the wind tunnel experiment (Figure 5.5), it is located \( h/2 \) downstream the last cube, which is 6\( h \) before the trailing edge of the heated surface. Velocity time-series are extracted from the points P1 to P4 and then used to compute spectra.

Schematics of the meshes of the L-LES and F-LES models are shown in Figure 5.17a and 5.17b respectively. Each mesh is made out of 4

Figure 5.17: Schematic drawing of the L-LES (a) and the F-LES (b) meshes along a vertical cut at \( y/h = 0 \). The top of the domain is not visible. A cell from level \( L_{n+1} \) is twice as small in every direction than one from \( L_n \).
5.6 Nested Simulations

<table>
<thead>
<tr>
<th>direction</th>
<th>$L_0$</th>
<th>$L_1$</th>
<th>$L_2$</th>
<th>$L_3$</th>
<th>$L_4$</th>
<th>$L_{4a}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_1, x_2$</td>
<td>$h/2$</td>
<td>$h/4$</td>
<td>$h/8$</td>
<td>$h/16$</td>
<td>$h/16$</td>
<td>$h/32$</td>
</tr>
<tr>
<td>$x_3$</td>
<td>$h/2.5$</td>
<td>$h/5$</td>
<td>$h/10$</td>
<td>$h/20$</td>
<td>$h/40$</td>
<td>$h/40$</td>
</tr>
</tbody>
</table>

Table 5.3: Size of the cells for each level of the LES meshes.

levels of refinement. $L_0$ is the base mesh level. Each level covers the entire streamwise and spanwise directions. Levels $L_1$ to $L_4$ extend vertically up to $8h$, $4h$, $0.6h$ and $0.16h$ respectively. Every mesh level is composed of rectangular cells. The cells of the level $L_{n+1}$ are twice smaller in each direction compared to the cells from the level $L_n$.

Figure 5.18 shows the vertical and horizontal cut of the S-LES mesh. The mesh is made out of 3 levels of refinement with $L_1$ as the base level. Every levels cover the entire domain horizontally, except $L_{4a}$, which only extends $4h$ in the spanwise direction. Levels $L_2$ to $L_{4a}$ stretch in the vertical direction to $4h$, $2.5h$ and $1.5h$ respectively. Table 5.3 shows the cell size for each level. In total, the LES without cubes is composed of 4.42 million cells. The L-LES and S-LES are made of 4.41 and 3.29 million cells respectively. According to Table 5.3, the smallest cells at level $L_{4a}$ measure $h/32 \times h/32 \times h/40$, which means $1.56 \times 1.56 \times 1.25mm$. To put those numbers into perspective, the PIV resolution for the configuration with cubes is $2.4 \times 2.4mm$. The reader should be careful with those numbers: even if the S-LES seems to
have a higher resolution than the PIV, the smallest eddy that it can capture spans across at least several cells. So the PIV still provides more accurate information with a higher spatial resolution.

The grid quality is evaluated with the $k_{res}$ criterion (Eq.4.1). According to Figure 5.19, the coarse grid of the LES without cubes is sufficient to resolve the flow well, with $k_{res} \in [0.96, 1.00]$. When the same grid is used in the configuration with cubes in the L-LES, since $k_{res}$ drops below 0.9 in the shear layer, and even below 0.8 in the critical parts near the cubes top. The finer grid of the S-LES shows the $k_{res}$ criterion higher than 0.98 in most of its domain with a small drop near the trailing edge of the last cube’s top.

With those grids, the $\langle y^+ \rangle$ of the first cell at the ground is equal to $\approx 2.2$ for all LES. At the cube walls, in the three spatial direction $i$, $\langle x_i^+ \rangle = 4.2$ for the L-LES and $\langle x_i^+ \rangle = 2.2$ for the S-LES. The $\langle x_i^+ \rangle$ of the cubes in the outer domain is quite high, as their top faces are sitting in the coarse level $L_2$.

5.6.2 Boundary conditions and solver setup

The F-LES and the L-LES use the same synthetic inflow generator as the LES described in Chapter 4 (proposed by Kornev and Hassel 2007). It generates a time-dependent turbulent inflow from the statistics and
lengthscale profiles shown in Figure 5.20. Those profiles are measured by the PIV, 3h upstream of the heated surface (above the mirror in Figure 5.3). From the PIV, only the streamwise and the vertical components of the velocity are available. The spanwise velocity is set to zero in the inflow generator. The three missing Reynolds stress have been reconstructed from the boundary layer data measured by Paterna (2015) in the same wind tunnel with the same ground roughness. The PIV integral lengthscale profile is computed from the PIV integral timescale, which is converted with the Frozen turbulent hypothesis. The measured integral lengthscale increases above \(z/h = 2\), which is unrealistic, because it is above the top of the boundary layer in a region where the Reynolds stress, hence the covariances, are zero. The unphysical values could be due to low frequency fluctuations in the wind tunnel flow. The lengthscale also shows a secondary peak close to the ground. Such a feature does not exist in the boundary layer profiles presented in literature (Moser et al. 1999). Turbulence might be triggered upstream of the measurement area, which locally...
generates larger structures. To remove the unphysical value above $z/h = 2$ and the secondary peak, the prescribed lengthscale profile is generated with a b-spline, fitting at best the PIV data.

The side boundaries in the F-LES and the L-LES are cyclic and the top boundary is symmetric. The gradient of velocity, temperature and pressure is set to zero at the outlet boundary. All the solid surfaces (ground and cubes if present) are set as a smooth walls. As the $y^+$ are small enough, wall functions are not necessary. The temperature of the ground is defined to match the desired $\Delta T$ and the cube temperature is set according to the measured data (Figure 5.11b).

The side boundaries in the F-LES and the L-LES are cyclic and the top boundary is symmetric. The gradient of velocity, temperature and pressure is set to zero at the outlet boundary. All the solid surfaces (ground and cubes if present) are set as a smooth walls. As the $y^+$ are small enough, wall functions are not necessary. The temperature of the ground is defined to match the desired $\Delta T$ and the cube temperature is set according to the measured data (Figure 5.11b).

The inlet, outlet, top and side boundaries of the S-LES are nested to the outer domain. Both the velocity and the temperatures of the L-LES are transfered through those boundaries. The blending distance is set to $d_w = h$ (Figure 5.16), with a relaxation time $\tau_r = 0.01$ s. The ground and the cubes of the S-LES are defined as smooth and wall-resolved, where the temperature is set similar to the L-LES.

To keep the Courant number $Co$ below unity, the timestep of the F-LES is set to 0.0012 s. The outer and the inner LES of the nested simulation have timesteps of 0.0012 s and 0.0003 s respectively. It gives a nested time ratio $N_{\Delta t}$ of 4 and by observing the grid in Figures 5.17 and 5.18, the average nested grid ratio around the cubes is equal to 3 in average.

The filtered Navier-Stokes equations (Eq.3.15) and the filtered conservation of energy (Eq.3.25) are solved in the F-LES and the outer LES. The buoyancy effects on the momentum are modeled with the Boussinesq approximation. Their nested counterparts are solved in the inner LES. The sub-grid scale (sgs) tensor $u''_i u''_j$ is modeled by the Smagorinsky-Lilly model proposed by Lilly (1992) and the sgs heat fluxes $\overline{u''_i T''_j}$ are approximated by Eq.3.26 and 3.27. The pressure-velocity coupling is done by the PISO algorithm.

### 5.6.3 Comparison with PIV, setup without cubes

Figure 5.21 shows a comparison between PIV and LES data of the mean streamwise velocity, the resolved 2D TKE and temperature difference. The velocity profiles of the LES (5.21a) are clustered together with only minor differences around $z/h = 0.1$. The measured velocity
Figure 5.21: Configuration without cubes: comparison between PIV and LES of the mean streamwise velocity, the resolved 2D TKE and temperature difference. The markers indicate the thermocouples.

profiles show an evolution of the shape with the temperature, which is not reproduced by the LES. The temperature profiles are visible in Figure 5.21c. The LES and PIV profiles match very well. For the case $\Delta T = 100\,K$ the LES predicts a slightly lower temperature of 1 K to 2 K in the upper part of the profile, above $z/h = 0.25$. In the magnified view in Figure 5.21c, the temperature profiles close to the ground are shown. The marker represents the measurement points (the thermocouples $TC_i$ of the TC-Fork). The LES is able to predict the temperature near the wall quite well, except for the very first thermocouple measurement. The measurements indicate a higher wall temperature gradient than the LES, which means that the simulation is likely to underestimate the heat transfer to the air, and therefore the buoyancy.

For the resolved $k_{2D}$, LES and PIV have quite different profiles. From the ground to $z/h = 0.25$, the peak of energy is well captured by the LES for every $\Delta T$. Above $z/h = 0.25$ only the LES case $\Delta T = 0\,K$ shows a good match with the PIV. The numerical simulations for the cases with $\Delta T = 60\,K$ and $\Delta T = 100\,K$ underestimate the energy.
above \( z/h = 0.25 \). This lack of energy is also visible in the two resolved Reynolds stresses \( \langle u'_1 u'_1 \rangle \) and \( \langle u'_3 u'_3 \rangle \) composing resolved \( k_{2D} \) in Figure 5.22a and 5.22b respectively. For the heated cases, the simulated Reynolds stress \( \langle u'_1 u'_1 \rangle \) is underestimated above \( z/h = 0.5 \). The underestimation is even stronger for the vertical turbulent fluxes \( \langle u'_3 u'_3 \rangle \). As explained in Section 5.5.1, the vertical turbulent fluxes are strongly influenced by buoyancy. The following points can explain this turbulent energy underestimation in the simulations:

- The amount of thermal energy extracted from the ground surface is likely to be too low in the LES, since the temperature gradient at the wall is lower in the LES than in the PIV. This can have a negative impact on the vertical turbulent fluxes by reducing the vertical fluctuations.

- The grid resolution might be too low, therefore it smears out the vertical turbulent fluxes too much. This can be improved by increasing the grid resolution in the vertical direction.
5.6 Nested Simulations

- The effect of buoyancy in the momentum $\text{sgs}$ model should be taken into account. With the current setup the raw Smagorinsky-Lilly model is used, but the model can be modified to include buoyancy effects (e.g. Langhans et al. 2012).

- The $\text{sgs}$ heat fluxes are modeled with Eq. 3.27. It can be improved by using a more sophisticated model, such as the one proposed by Lilly (1992).

According to the differences of wall temperature gradient between the LES and the PIV (Figure 5.21c), the first point seems to be the most important among the three.

Figure 5.23 shows the comparison between the PIV and the LES spectra for the four locations P1 to P4. For the lowest point P1 at

![Graphs showing energy spectra comparison between PIV and LES](image)

Figure 5.23: Configuration without cubes: comparison between PIV and LES of the energy spectra $E_{11}(\kappa)$ from cases $\Delta T = 0$ K and $\Delta T = 100$ K.
The PIV spectra from the cases $\Delta T = 0 \text{ K}$ and $\Delta T = 100 \text{ K}$ show similar energy content at every wavenumber. The LES spectra match the measurements very well up to $\kappa = 3 \cdot 10^1$, where the LES filtering starts. Similar observations can be made for the spectra at point P2. The LES predicts well for the large structures until the filter cut-off. As P2 is located in a coarser mesh region than P1, the cut-off starts earlier. At location P3 the PIV spectra are spread apart due to the buoyancy effects. They bring more turbulent energy to the flow at each wavelength. The energy content as well as the spread is also reproduced with good accuracy by the LES spectra. At the location P4, the effect of the buoyancy is even clearer on the PIV spectra. The energy content difference at small wavenumbers between the cases $\Delta T = 0 \text{ K}$ and $\Delta T = 100 \text{ K}$ is almost one order of magnitude. The LES is able to reproduce this larger difference qualitatively, but not quantitatively. The LES underestimates the energy content of the PIV for the heated cases, whereas the neutral case is well captured by the simulation.

5.6.4 Comparison with PIV, setup with cubes

Figure 5.24 shows a comparison between the PIV and the LES fields of instantaneous velocity magnitude $|u|$. Each row of figures shows the results for a given temperature difference. In each row, the left, central and right plot shows the PIV, the S-LES and the L-LES data respectively. The field of view is centered around the last cube. The effect of the grid is clearly visible by comparing the S-LES and L-LES rows. For each temperature difference, the S-LES shows finer structures in the cube wake. Above the cubes, the size of the structures is comparable between the inner and the outer LES. In the wake of the cube, the PIV fields and the fine-grained LES have similar fine turbulent features. Above the cubes, the PIV data shows more fine eddies than the S-LES, with a smoother transition from the wake region (below $z/h = 1$) to the freestream above. The PIV results show a clear evolution of the flow with increasing temperatures. The CBL gets thicker, with more turbulent structures. This evolution is visible in the S-LES and the L-LES, but with a lower intensity.

Figure 5.25 shows the mean streamwise velocity $\langle u_1 \rangle$. Both the inner
Figure 5.24: Configuration with cubes: comparison between the PIV and the LES fields of instantaneous velocity magnitude $|u|$. Field of view on the last cube only.
EXPERIMENT VALIDATION

Figure 5.25: Configuration with cubes: comparison between PIV and LES of the mean streamwise velocity $\langle u_1 \rangle$. Field of view on the last cube only.
and the outer LES predict the same mean contour, with negligible differences in the wake of the third cube. For the neutral case (first row of plots), both LES models can reproduce with a good accuracy the measured PIV field. For the heated cases (second and third row of plots) the simulations slightly underestimate the speed in the recirculation downstream of the first cube. The results show that the grids of the S-LES and the L-LES are sufficiently fine to capture the mean features. The problem appears in the higher order statistics, where the L-LES fails to predict them correctly.

The TKE comparison presented in Figure 5.26 shows some interesting differences between the PIV, the fine- and the coarse-grained LES. For the neutral case, the S-LES field matches the measurements with great accuracy. The turbulent shear layer downstream from the last cube has similar shape and intensity on both dataset. The interaction with the turbulent shear layer and the upstream face of the last cube is underestimated in the LES. In the convective cases, the shape of the shear layers before and after the last cube is well captured by the S-LES, but the intensity is generally too low: the PIV predicts a large area with high $k_2D$. Like in the neutral case, the L-LES of the heated cases cannot predict correctly $k_2D$, since its mesh is too coarse. The fine-grained grid of the S-LES therefore represents a clear advantage in that aspect. For the heated cases, the buoyancy has an indirect effect on $k_2D$ by increasing the amount of fluctuations. As seen in the configuration without cubes (Figure 5.22b), the numerical simulations underpredict the vertical turbulent fluxes, which are fueled by buoyancy. Even when the cubes are the main source of $k_2D$ (Section 5.5.1), buoyancy still has an influence and might explain the lower TKE levels in the turbulent shear layer as it is not modeled correctly.

Figures 5.27 and 5.28 show a comparison between PIV, S-LES and L-LES of the Reynolds stresses $\langle u'_1u'_1 \rangle$ and $\langle u'_2u'_3 \rangle$. Those two components are part of the 2D TKE and help one to understand the source of the discrepancies in $k_2D$.

For the neutral case, the $\langle u'_1u'_1 \rangle$ component of the Reynolds stress (first row in Figure 5.27) is very well captured by the S-LES. The high level pocket in the shear layer downstream from the last cube is similar in shape and intensity compared to the PIV measurements. The intensity of $\langle u'_1u'_1 \rangle$ in the shear layer from the second cube is slightly lower in the S-LES and its interaction along the upstream face.
Figure 5.26: Configuration with cubes: comparison between PIV and LES of the resolved 2D TKE $k_{2D}$. Field of view on the last cube only.
5.6 Nested Simulations

Figure 5.27: Configuration with cubes: comparison between PIV and LES of the Reynolds stress $\langle u'_1 u'_1 \rangle$. Field of view on the last cube only.
Figure 5.28: Configuration with cubes: comparison between PIV and LES of the Reynolds stress $\langle u'_3 u'_3 \rangle$. Field of view on the last cube only.
5.6 Nested Simulations

of the last cube is also underestimated. Interestingly, the shear layer produced by the second cube is transported above the top face of the last cube further downstream in the LES, which is not the case in the PIV. The L-LES has more difficulty to capture $\langle u'_1 u'_1 \rangle$ correctly. The shape of the downstream shear layer is correct, but the intensity is underestimated. The interaction of the second shear layer and the upstream face of the last cube is underestimated. There is almost no stress along this face.

For the heated case $\Delta T = 60$ K (second row in Figure 5.27), the S-LES predicts a similar $\langle u'_1 u'_1 \rangle$ pattern after the last cube compared to PIV. Near the ground, in the recirculation zone of the third cube, the intensity is slightly lower. The S-LES has more trouble to capture the shear layer from the second cube and its interaction with the third cube. The intensity is globally lower, especially at $z/h = 1$ and the lower streak along the upstream wall of the last cube is not very well predicted. As well as in the neutral case, the S-LES predicts a stronger transport of $\langle u'_1 u'_1 \rangle$ above the top face of the last cube. Surprisingly, the L-LES shows quite some good results in the shear layer from the last cube. Compared to the measured data, the intensity is at the right level and the shape is quite well reproduced. On the contrary, the level and pattern of $\langle u'_1 u'_1 \rangle$ before the third cube is poorly predicted.

The S-LES has more problems to reproduce the $\langle u'_1 u'_1 \rangle$ patterns in the heated case $\Delta T = 100$ K (third row in Figure 5.27). Downstream from the last cube, the shear layer from the simulation is smaller and with a lower intensity compared to the measurements. At the ground level, downstream of the last cube, the PIV shows a high stress pattern, which is not well predicted by the S-LES. The same observations can be made for the shear layer generated by the second cube. The L-LES shows worse results than the S-LES, both in shape and in intensity. In the L-LES, the peak value of $\langle u'_1 u'_1 \rangle$ downstream the last cube is 30% lower than in the PIV. Upstream the last cube, $\langle u'_1 u'_1 \rangle$ is even 50% lower compared to the PIV results.

Figure 5.28 shows the vertical turbulent fluxes $\langle u'_3 u'_3 \rangle$ measured by PIV and simulated by the nested LES. The PIV data (first row) show that the shear layer is the major contributor to $\langle u'_3 u'_3 \rangle$. Buoyancy also contributes to $\langle u'_3 u'_3 \rangle$. With a higher temperature difference, the intensity of the vertical turbulent flux increases near the ground, and also in the recirculation regions behind the second and the third cube.
In the neutral case, the S-LES can well predict the pattern of $\langle u_3' u_3' \rangle$ after the third cube, compared to the PIV. The shape is similar, but the intensity is slightly lower. Upstream of the last cube, the peak intensity is similar in the S-LES and the PIV, but its shape doesn’t spread that far upstream. The L-LES predictions for $\langle u_3' u_3' \rangle$ are clearly off: the intensity is too low and the shape is clearly wrong. In fact, the vertical turbulent fluxes generated by the cubes are simply not captured due to the too coarse grid in this region.

The vertical turbulent fluxes in the heated cases $\Delta T = 60\,\text{K}$ and $\Delta T = 100\,\text{K}$ are not correctly predicted by the S-LES (second and third line of Figure 5.28). For both cases, the fine-grained LES underestimates the peak values, whereas the patterns are correct.

Figure 5.29 compares the temperature difference $\Delta \langle T \rangle$ between the PIV and the nested-LES. Both S-LES and L-LES of the nested simulation predict the same temperature profile. They match well with the measured profile of the case $\Delta T = 60\,\text{K}$ but underestimate the temperature in the wake of the cube in the warmer case ($\Delta T = 100\,\text{K}$). This might be due to the Boussinesq approximation for modeling the buoyancy. This model is known to be correct for rather small temperature differences. In the configuration with cubes, a temperature
difference of $\Delta T = 100\,\text{K}$ might be too high. It would be interesting to run the nested simulation at different $\Delta T$ value to evaluate more precisely the limits of this approximation.

From the perspective of the nested simulation, the S-LES is able to reproduce the streamwise turbulent flux $\langle u'_1 u'_1 \rangle$ with good accuracy, but the prediction of the vertical turbulent flux $\langle u'_3 u'_3 \rangle$ is more problematic. As seen in Section 5.6.3, similar observations have been made regarding the flat surface F-LES. Since the model setup of the L-LES is similar to the F-LES (except for the cubes), they share the same limitation in their flat region, in which both underestimate the vertical velocity fluctuations. Therefore the S-LES received a too limited amount of vertical fluctuations and does not seem to be able to recover them. A modeling weaknesses can also explain the lack of $\langle u'_3 u'_3 \rangle$ in the S-LES: a too coarse grid in the vertical direction, the momentum sgs-model is unable to correctly model the influence of buoyancy, or the thermal sgs-model is too simple.

### 5.6.5 Spectra from PIV and LES

Figure 5.30 shows a comparison of the turbulent energy spectra $E_{11}(\kappa)$ between PIV and S-LES. The spectra are computed at the locations P1 to P4 (see Figures 5.15 and 5.16). At location P1, the S-LES predicts relatively well the measured spectra from $\kappa = 10^1\,\text{m}^{-1}$ to $\kappa = 4 \cdot 10^1\,\text{m}^{-1}$. At higher wavenumber, the energy drops quickly in S-LES due to the filter cut-off. The PIV spectra are not available below $\kappa = 10^1\,\text{m}^{-1}$. Indeed, the time series extracted from the PIV images are not long enough to capture the large, slow motion structures. At location P2, right in the shear layer, the largest turbulent structures from the S-LES have more turbulent energy than in the PIV. At higher wavenumbers, $E_{11}$ drops quickly in the simulation. It is not clear if the drop is due to the filter cut-off or to a wrong prediction of the energy. Like at the point P1, the energy starts to drop at relatively low wavenumbers, leaving the S-LES spectra with a very short $-5/3$ slope compared to the measured one. Higher in the boundary layer (P3, P4), the effects of the buoyancy starts to be visible within the spectra. As already seen in Figure 5.23, the heated case has more energy in all the
Figure 5.30: Configuration with cubes: comparison between PIV and S-LES of the turbulent energy spectra $E_{11}(\kappa)$. wavenumber ranges. The S-LES is able to predict this effect accurately, until $\kappa = 10^3 \text{m}^{-1}$.
5.7 Discussions and Conclusions

The wind tunnel experiment proposed in this chapter was designed to mimic a more realistic multiscale test case to validate the nesting procedure. The air flow above the heated surface was measured under two configurations, with and without cubes. Five cases were considered: a neutral condition and four CBL conditions from $\Delta T = 40\,\text{K}$ to $\Delta T = 100\,\text{K}$, with steps of 20 K in between.

In the configuration without cubes, the heated surface has a clear effect on the boundary layer compared to the neutral case. Above the linear part of the velocity profile (above $h/z = 0.2$ in Figure 5.7a), the profiles of the heated cases show a steeper gradient compared to the neutral case. The four profiles of the CBL show a slight clustering between $\Delta T = 40, 60\,\text{K}$ and $\Delta T = 80, 100\,\text{K}$. Among the three Reynolds stress components presented in Figure 5.8, $\langle u'_1 u'_1 \rangle$ and $\langle u'_1 u'_3 \rangle$ show a similar clustering effect, particularly important in the shear stress. The vertical turbulent fluxes $\langle u'_3 u'_3 \rangle$ do not show such an organization, but increase steadily with increasing temperature difference. This clustering can indicate a transition of flow regime at a given $\Delta T$ between 60 K and 80 K. There are two possible explanations for this clustering effect:

- The development of a laminar convective boundary layer can be divided in three regimes: a laminar region starting from the leading edge of the heated plate, a region with organized streamwise convective rolls and finally a chaotic turbulent region (Kudo et al. 2003). The CBL in this experiment does not start from a laminar boundary layer, therefore those three regions do not exist exactly as described. Nevertheless, a similar division in regions with different flow regimes are likely to exist in the measured setup. The length of those regions is likely to evolve with the temperature difference, hence the PIV measurements could have measured two different regimes. To fully understand the flow, the PIV measurements should be performed at various locations, from the leading to the trailing edge of the plate.

- The heated surface used in this experiment is finite. The effect of the edges can become more important above a given $\Delta T$. Moreover, the flow was measured close to the trailing edge of
the heated plate. Measurements near the edges could provide some interesting insights on the edge effects.

A combination of the above effects could be likely to be the source of this clustering effect.

The cubes have a large impact on the flow. High level Reynolds stresses are generated in the shear layer downstream of each cube. The rise of $\Delta T$ increases the area of high Reynolds stress, as well as their peak value. Interestingly, the Reynolds stresses are lower at $\Delta T = 40$ K compared to the neutral case. Above this value, the Reynolds stress increases with $\Delta T$. The CBL is thicker in the case $\Delta T = 40$ K than in the $\Delta T = 0$ K case. The velocity is lower at the cube height, hence the shear layer is weaker. The reason why the boundary layer is thicker in this case is not clearly understood.

In the configuration without cubes, the LES predicts the velocity and the temperature profiles well in all cases (neutral and heated). The $k_{2D}$ is correctly predicted near the ground in all cases, but under-predicted above $h/z = 0.5$. The Reynolds stress components $\langle u'_1 u'_1 \rangle$ and $\langle u'_3 u'_3 \rangle$ are also under-predicted above $h/z = 0.5$. It is likely due to the sgs-models used in the LES. The Smokorinsky-Lilly sgs-model used in the filtered momentum equation does not take into account convective effects. Several authors have proposed improved models, which can handle buoyancy more accurately (Langhans et al. 2012). The sgs-model of the filtered energy equation is proportional to $\nu_{sgs}$. More complex models can be used to improve the modeling of the sgs heat fluxes (Lilly 1992). LES is also found to be able to accurately reproduce the spectra until the filter cut-off.

A nested LES is used to simulate the configuration with cubes. The interaction between the inner and the outer domain are handled with the nesting procedure proposed in Section 3.5. The inner LES reproduces with great accuracy the velocity field measured in the wind tunnel, as well as the area of high 2D TKE. The peak values of turbulent energy are well predicted in the neutral and the $\Delta T = 60$ K cases, but under-estimated in the case $\Delta T = 100$ K. The temperature profile of the case $\Delta T = 60$ K is perfectly reproduced by the inner LES, whereas it under-estimates the temperature in the wake of the cube for the highest temperature difference $\Delta T = 100$ K. The under-estimated temperature and Reynolds stress at high temperature are due to the
5.7 Discussions and Conclusions

Boussinesq approximation for buoyancy. This approximation is known to be invalid with high temperature differences.

As a general conclusion, the S-LES model of the nesting procedure improves the results, especially the TKE. The grid of the S-LES in the vertical direction remains a critical aspect when buoyancy is important. The Boussinesq approximation for buoyant flow is valid for low $\Delta T$. For high $\Delta T$, the effects of the density variation become important, therefore compressible flow models should be used.
APPLICATION OF THE NESTED APPROACH TO A REAL CASE SCENARIO

In the previous chapters, the nesting procedure presented in Section 3.5 was used to simulate the flow in academic cases, made of several wall mounted cubes. Despite being a very simple representation of an urban topology, this arrangement of cubes reproduces the main geometrical features of common buildings, such as sharp edges and flat faces. The turbulent flow structures around cubes show similar features as real configurations, such as shear layers, recirculation and detached flows. Nevertheless, those simplifications hide some of the important characteristics of an urban flow immersed in a real Atmospheric Boundary Layer (ABL), like the varied topography and the land usage. Moreover the difference between the ABL turbulent scales and those generated by the buildings structures covers 1 to 2 order of magnitudes.

In this chapter, the nesting procedure is applied to a real case, where buildings are embedded in a full size ABL. In this situation, real means that the buildings, the topology and the land usage (ground roughness) are modeled in the numerical simulation as they exist. The physical inputs, such as wind speed, turbulence level and temperature, are selected to be close to reality.

The goal of this test case is to simulate the flow through the Hönggerberg campus of the ETH Zurich, under the influence of a typical neutral and unstable ABL. As the campus is built on a hill, a Large Eddy Simulation (LES) covering only the direct surrounding of the campus would miss the important flow modifications due to the hill itself. Therefore the nesting procedure is the right tool to achieve such a simulation.

The major steps to realize this realistic test case are now presented in detail. The capabilities and the limitations of every step are underlined and some possible improvements are proposed.
The Hönggerberg campus is one of the two campuses of the Swiss Federal Institute of Technology of Zurich - ETH Zurich. The campus sits on a shallow pass of the Hönggerberg hill (Figure 6.1). It is surrounded on its NW-SE axis -rise buildings rarely taller than 50 m. On the NE side of the hill stretches the relatively flat with a mixed rural-urbanized area of Affoltern. The city-center of Zurich is located \( \approx 4 \text{ km} \) NW of the campus. Zurich is a typical European city, with

![Figure 6.1: Implantation of the computational domain on the outskirts of the city of Zurich. Topography from the Federal Office of Topography - SwissTopo.](image-url)
densely packed low-rise buildings. The northern tip of the lake of Zurich is located roughly 5 km south of the campus.

The campus itself is a cluster of about 20 heterogeneous buildings as seen in Figure 6.2. It is relatively isolated from other constructions and surrounded by mostly green surfaces (forests or crops). The footprint of the campus can be approximated by a square of 600 m by 600 m. Most of the buildings have an horizontal extend of \( \approx 60 \text{ m} \times 60 \text{m} \), with the notable exception of the southern most building, with a comb-like shape, which has a footprint of \( \approx 100 \text{ m} \times 260 \text{ m} \). The average height of the buildings are \( \approx 25 \text{ m} \).

The flow through the campus is strongly influenced by the hill and the surrounding inhomogeneous roughness elements (forests, crops, city blocks). Therefore, standard ABL profiles (Richards and Norris 2011) cannot be used to feed a synthetic inflow generator, because they are derived on the hypothesis of flat and homogeneous terrain. A large computational domain is needed to take into account the effects of the roughness and topology on the ABL. But if the large domain includes well-resolved buildings, the timestep to account the very small cells near the buildings would have to be extremely small. A single domain LES would become computationally expensive and a

Figure 6.2: Geometry used for the ETH Hönggerberg campus. View from the south-west with late afternoon sun.
lot of computational time would be wasted in simulating the large turbulent structures of the ABL with an unnecessary small timestep. Therefore a nesting procedure is a very good candidate to use for this test case. The outer domain is dedicated to compute the ABL only, i.e. the roughness elements being parametrized by a wall-model. The inner domain computes only the flow through the campus, which is discretized by a well-resolved grid. The arrangement of both domains is shown in Figure 6.1.

6.2 Model setup and boundary conditions

6.2.1 Outer domain

As visible in Figure 6.1 and 6.3, the outer domain covers 4560 m in the NS direction and 3520 m in the EW direction. The Hönggerberg campus is located roughly in the middle of the outer domain and the campus buildings are parametrized by a wall model. The lowest topographic point included in the domain is at 391 m and the highest point is at 565 m. The average elevation of the campus is 524 m. In

Figure 6.3: Ground cover of the computational domain. Topography from the Federal Office of Topography - SwissTopo.
the vertical direction, the outer computational domain extends up to 3810 m, which is \( \approx 3350 \) m above the average ground level of the region. The domain is that high to avoid any strong blockage due to the hill. With such land cover, the domain covers a large part of the two forests surrounding the campus, as well as a part of the city located SW from it. The general dimensions of the domain are selected according to the best practice for LES of ABL (Moeng 1984; Sullivan et al. 1996; Noh et al. 2003; Botnick and Fedorovich 2008).

The outer computational domain is selected to simulate a neutral ABL with a height of 800 m Above Ground Level (AGL) and a mean wind direction from the South. This particular direction is selected to take into account the limitations of synthetic inflow generators. Indeed, inflow generators need the statistics and information on the eddy size (hence the lengthscale) to generate a turbulent inflow. Several methods are available to get these statistics and lengthscales:

- The statistics and lengthscales can be computed from standard profiles (Richards and Norris 2011) or similarity laws (Kaimal 1973; Holtslag and Nieuwstadt 1986).

- Statistics can be extracted from a mesoscale Numerical Weather Prediction (NWP) simulation. As all NWP models are based on the Reynolds Average Navier Stokes (RANS) equations, the turbulent lengthscales need to be approximated from algebraic models.

- The statistics and lengthscales can also be computed from a state-of-the-art LES of an ABL (Moeng 1984; Botnick and Fedorovich 2008).

In the first method, the profiles are constructed on the hypothesis of homogeneity and flat terrain. The second method provides realistic profiles but the resolution is quite poor. The operation NWP model which is used by meteoSwiss has a horizontal grid size of 2 km by 2 km and only a few cells are located in the ABL itself. The last method uses a LES to generate the statistics on a homogeneous and flat terrain. As it is a LES, the lengthscales can be directly computed from the data, without implying algebraic approximations. For this test case, a state-of-the-art LES of an ABL is used to generate the data for the synthetic inflow generator. Therefore the location of the inlet boundary
condition of the outer domain has to be located in a relatively flat area with a homogeneous ground cover. This explains the choice of the placement at the flat alluvial plain of the Limmat river. Details of the ABL-LES used to generate the inflow data are given in Section 6.5. For other wind directions, like a westward wind, data from a mesoscale NWP would be the most suitable approach as the statistics would suit the topology and the roughness inhomogeneities.

The terrain covered by the outer domain is inhomogeneous. To take into account the various roughnesses, it is split into 9 patches (see Figure 6.4). Every patch is modeled by the LES wall model as proposed by Schumann (1975) and described in more detail in Chapter 3, Eq.3.32. Table 6.1 gives the roughness length attributed to each patch. The roughness lengths have been chosen according the tables given by Davenport (1960) and Wieringa (1992). As the topology at the side boundaries is not the same, the east and west boundaries are set as a free-slip wall. The top boundary is also defined as a free-slip and a zero velocity gradient is applied to the north boundary (outlet).

As is common in weather simulations (ABL or mesoscale), the potential temperature $\Theta$ (eq.2.23) is used to describe the air temperature,
### 6.2 Model Setup and Boundary Conditions

<table>
<thead>
<tr>
<th>index</th>
<th>patch name</th>
<th>( z_0 )</th>
<th>description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>downtown</td>
<td>1.5</td>
<td>Large obstacles with open spaces half the size of the characteristic height</td>
</tr>
<tr>
<td>2</td>
<td>Höngg</td>
<td>1.0</td>
<td>Large obstacles with open spaces comparable to the characteristic height</td>
</tr>
<tr>
<td>3</td>
<td>Höngg forest</td>
<td>1.0</td>
<td>Mature forest</td>
</tr>
<tr>
<td>4</td>
<td>Affoltern</td>
<td>1.0</td>
<td>Large obstacles with open spaces comparable to the characteristic height</td>
</tr>
<tr>
<td>5</td>
<td>Chatzensee</td>
<td>0.5</td>
<td>Cultivated landscape with large obstacles separated by open space 5 to 10 time larger than the characteristic height</td>
</tr>
<tr>
<td>6</td>
<td>Zurich north</td>
<td>1.2</td>
<td>Same as Höngg, but slightly more packed</td>
</tr>
<tr>
<td>7</td>
<td>Chäferberg</td>
<td>1.0</td>
<td>Mature forest</td>
</tr>
<tr>
<td>8</td>
<td>campus front</td>
<td>0.25</td>
<td>low crops or pasture with scattered obstacles</td>
</tr>
<tr>
<td>9</td>
<td>campus</td>
<td>1.2</td>
<td>Same as Höngg, but slightly more packed</td>
</tr>
</tbody>
</table>

Table 6.1: Roughness length \( z_0 \) attributed to each patches. The patch index are shown in Figure 6.4.

As well as the surface temperature. \( \Theta \) is equivalent to \( T \) on the small vertical extends, such as buildings. In the following, the word *temperature* is used instead *potential temperature* for simplicity. The surface temperature of the campus patch is set to 340 K (\( \approx 67 ^\circ \text{C} \)). This quite high value is close to the simulated surface temperature in a cluster of buildings during a hot sunny day (Allegrini et al. 2015). The surface temperature of the other patches are set to 300 K for the neutral case and 306 K for the unstable case. 306 K is a common value used in literature to simulate a convective ABL on large scales. The temperature profile applied at the south boundary (the inlet) is extracted from the ABL-LES and used to generate the statistics for the synthetic inflow.
generator. A zero temperature gradient is applied to the east, west, north and top boundaries.

6.2.2 Inner domain

The inner domain is dedicated to simulate the turbulence flow through the campus. The ground footprint for the buildings, the land usage and the topology of the terrain are shown in Figure 6.5. The red box in Figure 6.3 shows its location inside the outer one. The inner domain covers 1000 m of terrain in the NS direction and 1100 m in the EW direction. The portion SW of the buildings is rather flat and covered by pastures. To the NE, the domain covers a portion of the slope towards the Affoltern area (see map in Figure 6.1). The campus itself is located in the middle of the domain. The top of the inner domain is located at 1200 m Above Mean Sea Level (AMSL), which is approximatively at 670 m AGL.

![Roughness and elevation maps](image)

Figure 6.5: Inner computational domain with the building footprints (light gray), roughness map (a) and AMSL elevation (b).

The ground is divided in patches of different roughnesses. The roughness length is given in Table 6.1. The buildings of the campus are resolved within the inner domain. Therefore the roughness length on the campus patch is forcefully set to \( z_0 = 0 \). The surface temperature for patches 3–4 and 7–8 are set to 300 K in the neutral case and 306 K in the unstable case. Patch 9 and the walls of the buildings are set to 340 K.
The south, east, west and top boundaries are the nested boundaries. They are coupled to the outer domain via the velocity and the temperature. The north boundary is not modeled as a nested boundary. The reason for this choice will be detailed in Section 6.7. Therefore, a zero velocity gradient and a zero temperature gradient are applied at the north boundary.

6.3 GRID

The grid of the outer domain is presented in Figure 6.6. The grid is made of a base layer $L_0$ and two refinement layers $L_1$ and $L_2$. Each layer covers the entire horizontal extent of the domain. The cells of each layer are cubical and their size is constant within any given layer. The transition between two consecutive refinement layers is sharp: a cell of the level $L_{i+1}$ is twice as small in all three directions than a cell from the level $L_i$. The grid of the inner domain is shown in Figure 6.7. It is composed of four level of refinements. The coarser levels $L_1$ and $L_2$ of the inner domain are the same as in the outer domain. The size of each level is given in Table 6.2.

<table>
<thead>
<tr>
<th>refinement level</th>
<th>$L_0$</th>
<th>$L_1$</th>
<th>$L_2$</th>
<th>$L_3$</th>
<th>$L_4$</th>
<th>$L_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>cell size in direction $x_i$</td>
<td>40</td>
<td>20</td>
<td>10</td>
<td>5</td>
<td>2.5</td>
<td>1.25</td>
</tr>
</tbody>
</table>

Table 6.2: Cell size for each refinement level composing the grids of the outer and the inner domain. The dimensions are given in meters.
Figure 6.7: Grid of the inner domain. a) is a vertical cut at $EW = 0\, \text{m}$ and b) is a terrain following surface at $z = 10\, \text{m AGL}$. Only the lowest part of the domain up to 900 m is shown. Level $L_1$ extends up to the top of the domain.

In total, the grids of the outer and the inner domain are made of 4.23 and 2.03 million cells respectively. Within the area of the campus, the mean grid size ratio $N_{\Delta x}$ is equal to $L_2/L_5 = 8$. 
6.4 SOLVER SETUP AND NESTING CHARACTERISTICS

The flow of the inner and the outer domain is simulated with a one-way, downscale nesting procedure described in Section 3.5. The outer LES is labeled as the Large scale LES (L-LES) and the inner domain is the Small scale LES (S-LES). The filtered Navier-Stokes equations with buoyancy (Eq. 3.6) are solved in both L-LES and S-LES. The Coriolis term, which rotates the flow at high altitude, is not included because the side boundaries cannot be defined as cyclic. This assumption is realistic when the studied area is at the ground level, as the rotation effect is significant only above \( \approx 200 \) m. The evolution of temperature is computed by the filtered conservation of energy equation (Eq. 3.25) in the L-LES of both cases. The S-LES solves the same set of conservation equations with the implicit blending procedure (Eq. 3.40b) added to the equations of conservation of momentum and energy. The blending distance is set to \( d_w = 60 \) m. The mesh of the inner domain near the nested boundaries is the same as the mesh in the outer domain. Hence new turbulent structures are not expected, therefore the blending distance can be relatively small. The Relaxation time is equal to \( \tau_r = 100 \) s. It is selected according to the integral timescale computed in the flat-terrain ABL used as a precursor for the Hönggerberg case (see next section). The sub-grid scale (sgs) stresses are modeled with the Smagorinsky-Lilly model (Lilly 1992) and the \( \langle u''_i T'' \rangle \) fluxes are modeled with Eq. 3.27.

The average Courant number \( C_0 \) is kept below one in the inner and the outer LES, which leads to timesteps of \( \Delta t^L = 0.6 \) s and \( \Delta t^S = 0.06 \) s for the L-LES and the S-LES respectively. With a timestep ratio of \( N_{\Delta t} = 10 \) and a grid ratio of \( N_{\Delta x} = 8 \), the nesting is quite strong, therefore the gain in computational time is important. To estimate the gain, we can imagine a single-domain LES. It would have the same land cover as the L-LES, but with the campus being building-resolved. The grid would be similar to the L-LES with a local refinement around the buildings similar to the S-LES. With this configuration, the single-domain LES would have a grid of 5.99 million cells and a timestep equal to \( \Delta t^S = 0.06 \) s to keep \( C_0 < 1 \). With those numbers, the wall-clock \( \Delta t^c \) ratio would be equal to \( \Delta t^S / \Delta t^N_c = 2.44 \) (Eq. 3.45), which means that the nested simulation is 2.44 times faster to compute than
a single-domain simulation. In this test case, the saving in term of computational time is mainly due to the large difference on timestep.

The pressure-velocity coupling is handled with the Pressure Implicit with Splitting of Operator (PISO) algorithm, with two pressure correction loops. The momentum and the equation conservation are solved with a preconditioned bi-conjugate gradient (PBiCG) solver and the pressure equation uses a geometric-algebraic multi-grid (GAMG) solver.

6.5 Generation of the inflow data

A time-dependent, fully turbulent velocity field must be provided to the south boundary of the outer domain as inflow. To do so, the synthetic turbulent inflow generator proposed by Klein et al. (2003) is used. The generator has been simplified by Xie and Castro (2008) and is available as an OpenFOAM implementation (Vonlanthen and Immer 2015a). The main interest of this generator compared to the one used previously in Chapters 4 and 5 is the possibility to define the nine lengthscales. As the turbulent structures in a Convective Boundary Layer (CBL) are known to be strongly anisotropic in the vertical direction (Moeng et al. 2007), this is an advantage.

The profiles for the inflow generator have been extracted from two state-of-the-art LES for a Neutral Boundary Layer (NBL) and a CBL over a flat and homogeneous terrain (constant roughness). The numerical domain of both simulations cover a flat terrain of 3 km × 3 km with a vertical extend of 1.6 km. The grid is composed of three layers. The first layer extends from the ground to 400 m and is made of cubic cells each with a size of 10 m. The second layer is stacked above the first one, up to 1000 m with each cubic cell of 20 m in size. The upper most layer fills the domain up to the top boundary with 40 m sized cubic cells.

The ground boundary condition is parametrized with the wall-model proposed by Schumann (1975). The roughness length $z_0$ is constant over the surface and set to $z_0 = 0.5$. The side boundaries are cyclic and the top boundary is modeled as a free-slip wall. At the startup of both LESs, the vertical profile of mean potential temperature $\langle \Theta \rangle$ is set to 300 K until 750 m, then followed by an inversion layer of
100 m with a positive temperature gradient of 0.08 K m$^{-1}$. Above the inversion, the temperature increases by 3 K per km. The middle of the inversion is at 800 m and defines the height of the ABL. The ground temperature is set to 300 K for the NBL and 306 K for the CBL. The flow in both simulations is driven by a constant pressure gradient. As it will be shown in the next section, the heat transfer from the ground has an important effect on the velocity, covariance and lengthscale profiles in the unstable case. To have a comparison as fair as possible between the neutral and unstable nested cases, the pressure gradient is set to provide a mean wind speed of 5 m s$^{-1}$ at 200 m. Fair in the sense that only a limited amount of parameters should change between the two simulations.

For both simulations, the filtered Navier-Stokes equations with buoyancy (Eq.3.6) and the filtered conservation of energy (Eq.3.25) are solved by the OpenFOAM ABL solver proposed by Churchfield et al. (2010). The temperature $T$ is replaced by the virtual temperature $\Theta$ in the filtered energy equation. The Smagorinsky-Lilly model (Lilly 1992) is used to parametrize the sgs stresses and the $\langle u''T'' \rangle$ fluxes are modeled with Eq.3.27. The Coriolis term has an important effect on the flow direction in the higher part of the ABL. An Ekman spiral (Ekman 1905) forms in the ABL and the flow direction between the lower and the upper part of the ABL can change up to 30deg. Nevertheless, the Coriolis term is not included in the momentum equation for the following reasons:

- The inflow data generate by the flat terrain LES will be use in the inflow generator and need to take into account its limitations. Indeed, in its current formulation, inflow generators cannot recreate a turbulent flow with a changing streamwise flow direction.

- The simulation domain of the Hönggerberg campus include the hill of Hönggerberg. As the hill is obviously not symmetric, the sides of the domain are also not symmetric. Therefore a cyclic boundary condition on the Hönggerberg domain is not applicable. Without the cyclic condition, a rotation due to the Coriolis force in the higher part of the ABL can not be handled.
The Coriolis force acts only in the upper part of the ABL. As this case study is interested mainly on the effect of the ABL on the buildings, the absence of Coriolis term should not be problematic.

Both LESs simulate the ABL 20 h of physical time. The last 5 h are used to compute the statistics of the flow, as well as the lengthscale.

6.5.1 Results

The vertical mean velocity $\langle u_i \rangle$ and temperature profile $\langle \Theta \rangle$ are shown in Figure 6.8. The CBL is 100 m higher than the NBL. In the LES, nothing stops the CBL from growing, as the turbulence is always fed by the warm ground. In reality, the growth of an CBL would stop in the late afternoon, when the solar forcing reduces. The mixing effect of the CBL is also clearly visible. The streamwise velocity $\langle u_1 \rangle$ of the CBL has a very sharp gradient near the ground, and then stays almost constant until the top of the ABL. The same occurs for the
temperature: after a strong gradient near the ground, the temperature remains constant up to the ABL top. The velocity profile of the NBL is closer to the well known log-law profile, with a smooth evolution of the speed with respect to the height. As expected, the location of the inversion (800 m) and its strength (0.08 K m$^{-1}$) remain constant in the NBL simulation. The inversion acts as a strong barrier, which suppresses the turbulence in the free atmosphere above the ABL.

The turbulent structures in the CBL are generally larger than in the NBL. Large vertical structures develop in the CBL and are clearly visible in a vertical, spanwise cut plane as shown in Figure 6.9. In the CBL, the vertical velocity fluctuations $u'_3$ are organized in large vertical structures, which can span over 400 m in the $z$ direction and the $y$ direction. The turbulent structures of the NBL, are much smaller, and evenly distributed in the ABL. Above 800 m in the NBL and

![Figure 6.9: Vertical velocity fluctuations $u'_3$ on a vertical, spanwise cut plane. Comparison between the NBL and the CBL.](image)
900 m in CBL, the turbulent structures disappear. It is the effect of the temperature inversion layer (cold to warm), which kills the turbulence. The Reynolds stresses and the velocity-temperature covariances as shown in Figure 6.10. In the CBL, the ABL keeps growing and pushes

![Diagram](image)

Figure 6.10: Vertical profile of the Reynolds stress $\langle u'_i u'_j \rangle$ and the velocity-temperature covariance $\text{cov}(u \Theta)$. Comparison between the neutral (dashed lines) and the unstable ABL (solid lines).

the inversion higher. Therefore covariances of the CBL from $\approx 750$ m to $\approx 1000$ m are not valid, as the flow in this layer is statistically non-stationary. The buoyancy mainly influences the three diagonal components of the Reynolds stress tensor. In the CBL, $\langle u'_i u'_i \rangle$ is roughly twice as big than in the NBL. The peak is located at a similar height, but with higher intensity. The buoyant effects are even stronger on the component $\langle u'_2 u'_2 \rangle$, which becomes more than four times larger than in the unstable case. The peak value equals $0.45 \text{ m}^2/\text{s}^2$ whereas it is only $0.18 \text{ m}^2/\text{s}^2$ in the neutral case. Higher up, the unstable $\langle u'_2 u'_2 \rangle$ keeps decreasing, but with values still four times higher than in the neutral case. The most interesting effects of buoyancy are visible on the vertical turbulent flux $\langle u'_3 u'_3 \rangle$. Whereas this Reynolds stress component stays rather small in the neutral case, it becomes one of
the most important components in the unstable case. The peak is shifted to 300 m and equal to 0.5 \( m^2/s^2 \). In the neutral case, the peak of \( \langle u'_3 u'_3 \rangle \) is reached at 50 m, with a value of 0.08 \( m^2/s^2 \), hence more than six times smaller than in the unstable case.

From each ABL, nine lengthscales \( L_{i,j} \) can be extracted. \( i \in [1, 2, 3] \) represents the spatial direction and \( j \in [1, 2, 3] \) the velocity component. For example, the lengthscale \( L_{12,1} \) can be interpreted as the mean size in the spanwise direction \( x_2 \) of a cluster of streamwise velocity \( \bar{u}_1 \). The term cluster can somehow be replaced by eddy, even though an eddy is generally pictured as a vortex with a rotating motion. The lengthscales of the NBL and the CBL are shown in Figure 6.11.

![Figure 6.11: Vertical profile of the lengthscales \( L_{i,j} \), where \( i \) is the spatial direction and \( j \) the velocity component. Comparison between the CBL (solid lines) and the NBL (dashed lines).](image)

In the streamwise direction \( (L_{11,i}) \), the lengthscale \( L_{11,1} \) steadily grows with the altitude, whereas \( L_{11,2} \) and \( L_{11,3} \) stay relatively constant. In the CBL, \( L_{11,1} \) and \( L_{11,2} \) are strongly affected in the first 150 m above the ground. Buoyancy has a smaller effect on \( L_{11,3} \), which grows linearly with the elevation, like in the NBL but with a more important
growth rate. In this lower part of the ABL, the structures are bigger in the spanwise direction than in the other directions, whereas the structures are always oriented along the flow in the NBL. Similar trends can be seen for the three lengthscales in the spanwise direction ($L_{ij}$). In the NBL, they all grow linearly with the altitude. In the CBL, $L_{i1}$ and $L_{i2,j}$ reach a first peak value around 100 m and then remain relatively constant up to 400 m. Higher up, $L_{i1}$ and $L_{i2,j}$ start to grow again. The effects of buoyancy are quite different in the vertical direction ($L_{i3,j}$). The lengthscales $L_{i3,1}$ and $L_{i3,2}$ are marginally modified by the convection. The shape of their curves are slightly modified, but the mean value remains similar to their counterpart from the neutral case. Major modifications occur on the $L_{i3,3}$. In the CBL, the peak value of $L_{i3,3}$ is reached at around 250 m AGL, with a typical size of 280 m.

The statistics presented in Figures 6.8 and 6.10, as well as the lengthscales of Figure 6.11 are used by the turbulent inflow generator in the nested simulations of the Hönggerberg campus. The inversion layer, and it’s behavior over the hill of Hönggerberg is not well known (does it follow the ground or not?) and would depend on large mesoscale features which are not resolved in the outer LES therefore the statistical profiles are simplified and the inversion is removed. They are presented in Figure 6.12. The lengthscales profiles used in inflow generator are shown in Figure 6.13. The profiles are simplified by piecewise linear curves to account the for the capabilities of the inflow generator. To reproduce the shape transition from the turbulent ABL the laminar region aloft, the lengthscales set to zero above $z = 770$ m for the NBL and $z = 800$ m for the CBL.

At the time those simulations were performed, the inflow generator was not able to create a turbulent temperature field. Therefore only the mean temperature profile is enforced in the CBL simulation of the Hönggerberg campus. Nevertheless, the velocity-temperature covariances stay very small in the ABL, so the lack of temperature fluctuations at the inlet of the nested simulations should not be problematic. Very recently, a new turbulent inflow generator for scalars (e.g. the temperature) has been proposed by Immer (2016). Such a generator could be used in future LESs of ABL to take into account the temperature fluctuations or any other scalar fluctuations.
Figure 6.12: The neutral ABL profiles (a) and The unstable ABL profiles (b) used in the inflow generator of the nested-LES of the Hönggerberg campus.
Figure 6.13: Lengthscale profiles used in the inflow generator for the nested-LES of the Hönggerberg campus. NBL lengthscale (a) and CBL lengthscale (b).
6.6 RESULTS

In the following sections, the results of the inner and the outer LES of the nested simulations are presented with cut plane images and vertical profiles. All horizontal dimensions are given according to the coordinate system [SN,WE] defined in Figure 6.1. The results extracted from terrain-following cut-planes are oriented like a map, hence north on the top and west on the left. In those images the flow goes from the bottom to the top (south to north).

6.6.1 Large scale LES

As seen in the flat terrain simulation used to generate the inflow statistics, buoyancy has a large effect on the shape and size of the turbulent structures. Figure 6.14 shows the vertical velocity fluctuations $u'_3$, on a vertical cut-plane aligned with the axis SN and cutting the outer domain of the NBL and CBL in the middle, at $EW = 0$ m (see Figure 6.3). The blue part of the ground line indicates the location of the campus.

Figure 6.14: Vertical velocity fluctuations $u'_3$. Streamwise vertical cut-plane at $E \rightarrow W = 0$ m. The blue part of the ground line indicates the location of the campus.
pus. From the inlet of the domain to approximatively $SN = 2800\, \text{m}$, the differences between the mechanically driven turbulence (neutral $\text{ABL}$) and the buoyancy driven turbulence (unstable $\text{ABL}$) are clearly visible. The $\text{CBL}$ is populated with vertically elongated structures with upstream fluctuations. Those structures, generally known as thermals, extend from the ground to the top of the $\text{ABL}$ ($\approx 900\, \text{m}$ height) and are 100 to 200 m wide in the streamwise direction. The turbulent structures in the $\text{NBL}$ grow with the elevation, without showing a real anisotropy in shape. In the neutral case, roughly 500 m after the campus patch, thermal-like structures start to develop. 1000 m after the campus, those new thermals are already 400 m tall, which is roughly half of the total $\text{ABL}$ height. Those structures found their origin with the heating of the air, flowing over the campus area. In the $\text{CBL}$, the added energy from the campus patch does not significantly affect the turbulent structures in the upper part of the $\text{ABL}$.

Figure 6.15 shows the vertical velocity fluctuations $u'_3$ on the terrain-following plane, placed at 100 m AGL. The location of the campus is highlighted in gray. In the $\text{NBL}$, the turbulent structures of vertical fluctuations are elongated in the streamwise direction and stay rather thin in the spanwise direction. In the wake of the campus, the vertical fluctuations become more intense and the shape of the structure changes. The newly created structures are similar, although smaller, than the buoyant eddies visible in the unstable case. Large buoyant structures are visible in the $\text{CBL}$ (right plot of Figure 6.15). They can extend over 1000 m in the streamwise direction and 200 m in the spanwise direction. As already observed in Figure 6.14 the effect of the thermal plume produced by the patch of the campus is not clearly visible.

The evolution of the $\text{ABL}$ statistics of the vertical profiles through the outer domain is presented in Figures 6.17 and 6.18. The data are extracted for five vertical lines L1 to L5, which are located on the vertical streamwise cut-plane $EW = 0\, \text{m}$ (see Figure 6.16). In the those figures, the profiles are shown with respect to the AGL elevation. The three first lines are located upstream the campus, with the third one on the windward slope of the hill. The fourth line is placed in the middle of the campus patch and the last line is located on the leeward side of the hill.
6.6 Results

Figure 6.15: Vertical velocity fluctuations $\overline{w_3}'$. Terrain-following cut-plane at 100 m AGL. The location of the campus is highlighted in gray.

Figure 6.16: Location of the vertical lines used to extract the statistical profiles.

The evolution of the NBL and the CBL mean streamwise velocity profiles $\langle \overline{u_1} \rangle$ along the lines L1 to L5 are given in Figure 6.17. From the inlet line L1 to line L2, the mean velocity profiles do not show much evolution, which is expected according to the flat topology and the homogeneous land usage of the alluvial plain. On the windward side of the hill, at line L3, the flow accelerates, especially in the first 50 m.
above the ground, where it gains about 1 m s$^{-1}$ in both cases. Above the campus patch, at line L4, the profile of the neutral case is similar to the one of the unstable case up to a height of 150 m AGL. This is likely due to the acceleration phase experienced on the windward side of the hill. On the leeward of the hill (line L5), the NBL profile has the typical characteristics of an unstable ABL; a strong velocity gradient at the ground followed by a range of almost constant velocity. Above
a height of 200 m in the AGL, the velocity profile of the neutral case is unperturbed by the convective plume of the campus.

The profiles of the vertical turbulent fluxes are presented in Figure 6.18. The profile of L1 shows the statistics prescribed by the turbulent inflow generator. Line L2 is located 800 m downstream from the first line. The curves at L1 and L2 for the neutral case are similar, whereas the intensity of $\langle u'_3 u'_3 \rangle$ in the unstable case decreases by $1/4$ between the first and the second line. Between those two lines, the terrain
The application of the nested approach to a real case scenario is flat (alluvial plain) and its land usage is modeled by a constant roughness of $z_0 = 1.5$. The statistics imposed by the inflow generator were generated from the precursor LES presented in Section 6.5.1, which models the ground with a roughness of $z_0 = 0.5$. It is therefore expected that the bottom part of the profile evolves. In this case, the lower $\langle u'_3 u'_3 \rangle$ above a height of 150 m AGL are due to turbulence reconstruction. Indeed, the turbulence generated at the inflow matches the required statistics, but it is still synthetic turbulence (hence, non physical) and needs a certain distance to develop. According to Immer (2016), two to three ABL heights are needed for a complete reconstruction of turbulence over a flat plate. In this case, the hill shortened this distance, as the topology will trigger new turbulent structures, which enables the possibility to use a shorter inlet fetch. On the windward slope of the hill (line L3), $\langle u'_3 u'_3 \rangle$ increases in the region below a height of 200 m AGL. Whereas the increase due to mechanical turbulence and the slope (neutral case) stays very small, and the effect of the buoyancy is much more pronounced (unstable case). Above the campus (line L4), the profiles are relatively similar to the one visible on the line L3. Downstream from the campus patch the effects of the buoyant plume are clearly visible. From 0 m to 100 m, the gradient of $\langle u'_3 u'_3 \rangle$ is similar for the NBL and the CBL. Above a height 100 m AGL, the unstable ABL shows higher vertical fluxes than the neutral ABL, and those fluxes remain higher in the rest of the ABL.

The effects of the buoyant plume developing downstream of the warm campus patch are important. In the plume, the neutral ABL profile develops the characteristics of a typical unstable ABL: well mixed velocity profiles, large buoyancy-driven turbulent structures and strong vertical turbulence fluxes. 1000 m from the release location, the NBL and CBL are clearly affected by the buoyant plume up to a height of $\approx 400$ m AGL (last plot of Figure 6.18). The plume is likely to affect the flow for several kilometers after its starting point. In a real situation, similar plumes will develop from buildings located upstream from the campus and will affect the Hönggerberg campus itself. This shows that all the elements surrounding an area of interest may play a significant role and produce a buoyant effects, even the ones located several kilometers upstream. For simplicity, the heating up of the area upstream the region of interest is not modeled.
6.6.2 Small scale LES

The S-LES computes the flow in the inner domain. The grid at the outskirts of the inner domain is similar to the grid of the outer domain (see Figure 6.7 and 6.6). Therefore the development of new turbulent structures is not expected in this region. Closer to the buildings, the grid is 8 times finer in every direction than the outer domain grid in order to be able to capture the small turbulent structures triggered by the buildings. Those new small eddies can be easily identified in Figure 6.19, which shows the vertical fluctuations on a vertical-cut plane ($EW = 0 \text{ m}$). The new structures have roughly the size of the buildings. They form a roughness layer (see Figure 2.6 in chapter 2), which extends 2 to 2.5 times the mean building height, $z_b = 20 \text{ m}$ above the ground. The characteristic speed deficit of such a layer can be seen in Figure 6.20. The roughness layer begins to develop from the first buildings and slowly grows until the downstream edge of the campus ($SN = 2820 \text{ m}$), where it reaches a depth of $\approx 3z_b$. After the last building, the growth rate of the roughness sublayer

![Image of vertical velocity fluctuations](image_url)
Figure 6.20: Mean streamwise velocity $|\langle \bar{u} \rangle|$ on the streamwise vertical cut-plane at $E \rightarrow W = 0$ m.

increases due to the downward slope of the hill, which acts as a divergent. Interestingly, both CBL and NBL have a similar roughness layer. The only differences is that the wake in the CBL case is slightly thicker. Above the roughness layer, the outer Layer (Figure 2.6) is visible in Figure 6.19. This layer is populated by structures of the large scale ABL. In the unstable case, typical elongated clusters of vertical fluctuations start directly above the roughness layer and extend up to the top of the domain (not visible in the picture).

Inside the roughness layer, the mean velocity magnitude field $|\langle \bar{u} \rangle|$ of the neutral and the unstable case are almost identical, as it can be seen in Figure 6.21. Within the campus area, the mean velocity magnitude between the building is 1 m s$^{-1}$ to 2 m s$^{-1}$ in average. The recirculation pockets and the areas of higher velocity are very similar between the two cases. The impinging velocity at $SN = 2350$ m (bottom part of the plots in Figure 6.21) is almost identical in both case, which explains the similar velocity field within the campus area.

Looking back at larger scales (Figure 6.17), the velocity profile near the ground is almost similar at the evaluation line L4 (located on the
Figure 6.21: Mean streamwise velocity $|\langle \bar{u} \rangle|$ on the terrain-following cut-plane at 20 m AGL. The campus buildings are displayed in gray.

campus. Moreover, the grid of the outer domain is made of 10 m tall cells. This means that small variations of velocity in the first 20 m, which would be important at the building level, are simply not captured by the outer domain, and therefore the impinging velocities in the inner domain are identical in both cases. To solve this issue, the upstream part of the inner grid can be refined near the ground, which would help with the generation of more realistic wind fluctuations between 0 m to 20 m AGL. The wind velocity in this layer is especially important for wind comfort assessment.

Figure 6.22 shows the potential temperature $\langle \Theta \rangle$ and the potential temperature difference $\Delta \langle \Theta \rangle$ on a terrain-following cut-plane at 20 m AGL. The mean temperature upstream from the campus (at $SN = 2350$ m) is used as a reference to compute $\Delta \langle \Theta \rangle$. As expected, the air temperature on the campus is about 3 K higher for the CBL compared to the NBL (third plot in the upper row of Figure 6.22). In terms of temperature difference (lower row of Figure 6.22), both cases show similar patterns. In the central part of the campus, the air is 1.25 K to
1.75 K warmer than the air outside of the campus. It denotes a small heat island effect as is usually the case in an urbanized area.

The stability of the ABL has more consequences on the Reynolds stresses. Figure 6.23 shows the horizontal turbulent fluxes $\langle u'_1 u'_1 \rangle$. Plumes of high $\langle u'_1 u'_1 \rangle$ are mainly generated at the leading edges of the upstream buildings indicated by B1 and B2 in both the neutral and unstable cases. Inside the campus, the $\langle u'_1 u'_1 \rangle$ turbulent fluxes are higher in the unstable case than in the neutral case. In the wake of the campus, there is an important build up of $\langle u'_1 u'_1 \rangle$. It is likely related to the increasing growth rate of the roughness layer visible in Figure 6.20.

The vertical turbulent fluxes $\langle u'_3 u'_3 \rangle$ visible in Figure 6.24 are also mainly generated at the leading edge of the upstream buildings B1 and B2. Those patterns of high $\langle u'_3 u'_3 \rangle$ show larger values in the unstable case. More generally, the intensity of the vertical turbulent fluxes inside the campus are higher in the CBL case than in the NBL.
Figure 6.22: Potential temperature data on a terrain-following cut-plane at 20 m AGL. The mean potential temperature on the line $SN = 2350$ m is used as a reference to compute $\Delta \langle \Theta \rangle$. The campus buildings are displayed in gray.
Figure 6.23: Horizontal turbulent flux \( \langle u'_1 u'_1 \rangle \) on the terrain-following cut-plane at 20 m AGL. The campus buildings are displayed in gray.

Figure 6.24: Horizontal turbulent flux \( \langle u'_3 u'_4 \rangle \) on the terrain-following cut-plane at 20 m AGL. The campus buildings are displayed in gray.
6.7 Discussion

In this test case some important and realistic features existing, such as topology and land usage, are reproduced. As the area of interest is located on a hill, a standalone, a small scale LES (e.g. the S-LES alone) is not realistic. Some modifications of the flow field due to the hill would not be predicted, such as the flow acceleration visible in Figure 6.17. However the usage of a large scale domain, like the outer domain, with a local mesh refinement at the location of the inner domain would make the simulation 2.44 times more time consuming (see Section 6.4), therefore hardly applicable. The nesting procedure presented in this thesis shows its high potential in such truly multiscale flows. In one nested-LES, both the large and small scales are simulated, as well as the downscale interactions.

As described in Section 6.4 the S-LES is coupled with the L-LES via the south, east, west and top boundaries, but the north boundary (the outlet) is not coupled. Figure 6.25 shows the mean velocity magnitude in the neutral case for the S-LES, the L-LES and a third LES. The third simulation has the same setup as the L-LES, but with buildings from the campus only crudely resolved. The grid around the buildings is refined to level L3 (see Tab.6.2), which means a cell size of 5 m at the wall. The idea of this simulation is to see which improvement would be achieved when a better approximation for the buildings is used. Going back to Figure 6.25, the roughness layer is clearly missing in the wall-modeled L-LES compared to the S-LES. It is somehow expected, because the wall-models used in LESs are designed to provide the proper surface stresses and fluxes to the outer layer of a boundary layer (e.g. an ABL), and the flow through the roughness elements is not a concern at such scale. The crudely building-resolved LES shows a better prediction of the roughness layer compared to the wall-modeled L-LES, showing a correlation much closer to the results given by the S-LES. The thickness of the roughness layer is rather well reproduced, but the decrease in velocity is underestimated in the wake of the campus. From these results, the second L-LES seems to be a good candidate to serve as a fully coupled outer domain. Unfortunately, resolving the buildings, even coarsely, implies a reduction of the timestep by a factor of six compared to the wall-modeled L-LES. In other words, a computational time of a
Figure 6.25: Mean streamwise velocity $|\langle \bar{u} \rangle|$ on the streamwise vertical cut-plane at $E \to W = 0$ m. Comparison of the results between the S-LES, the L-LES and a second L-LES with only crudely resolved buildings.

nested simulation with the buildings resolved in a L-LES would be much longer compared to the nested setup proposed in this chapter.

On a larger scale, the effects of the wake downstream from the campus buildings can be seen in Figure 6.26. According to the building resolved L-LES, the wake affects the flow field up to 1.5 km after the campus location. The wall-modeled L-LES predicts neither the roughness layer, nor the far-field wake. The leading edge of the campus is located only 500 m downstream of the last buildings on the SW slope of the Hönggerberg hill (see map on Figure 6.3). Those buildings upstream are not resolved in the L-LES, but they are likely to
Figure 6.26: Mean streamwise velocity $|\langle \bar{u} \rangle|$ on the streamwise vertical cut-plane at $E \rightarrow W = 0$ m. Comparison of the results between the wall-modeled and the building resolved L-LES.

generate a roughness layer. This roughness layer may interact with the campus. The wall model used in both L-LESs is not able to reproduce the roughness layer with a reasonable level of accuracy, which can affect the quality of the results for the S-LES, especially in a more integrated situation.

A one-way downscale nested simulation relies heavily on the capabilities of the outer domain to simulate the effects of the parametrized elements (the buildings in this test case) on the flow, which are then resolved within the inner domain. As the area of interest is always located in the first 100 m above the ground, this layer should be reasonably predicted by a computationally efficient wall model. Presently, roughness models for LESs cannot reproduce the mean effects of the roughness layer, but better models can be found in operational NWP. However, all those NWP are RANS based solvers, therefore their models can not be directly applied to the LESs, but can be used as a starting point. For example, Martilli et al. (2002) propose an urban exchange
parametrization model for the mesoscale NWP's, where a urban area is statistically approximated as porous media. Such a model could serve as a basis for new LES wall functions, where the roughness layer is correctly reproduced.

6.8 CONCLUSION

The nesting procedure proposed in Chapter 3 is successfully applied to a real test case, where the entire ABL is modeled by the outer coarse-grained LES and the buildings of interest are resolved by the inner fine-grained LES. The flow around the buildings is accurately reproduced, as well as their effects on the lower layer of the ABL. The nesting procedure is better able to produce high quality results for a fraction of the computational time required by a single domain LES with similar land cover and grid refinement. In the case presented in this chapter, the nested-LES is $\approx 2.5$ times faster than an equivalent single domain LES.

The main issue for such one-way downscale nesting procedure is the capability of the outer domain to reproduce the effects of the parametrized roughness elements on the flow with a reasonable level of accuracy. Actual LES surface models are only designed to simulate the effects of the ground on the outer layer of the ABL. New models with a better representation of the roughness layer should be developed for an efficient use of nested-LES and more generally for building resolved LES of urban configurations.
CONCLUSIONS AND OUTLOOKS

This chapter summarizes the research carried out in this thesis. The main results of the numerical validation, experimental validation and the test case are presented in the first section. The second section presents the mean contribution to the research field and the last section proposes several perspectives for further work.

7.1 SYNTHESIS

This thesis presents a novel approach to tackle the problem of multiscale interactions in the urban microclimate. The typical energy containing turbulent structures found in Atmospheric Boundary Layer (ABL) are 100 m to 1000 m in size, while the turbulent eddies generated by buildings extend from 2 m to 20 m. The one-way, downscale nested Large Eddy Simulation (LES) to LES proposed in this thesis allows to resolve this wide range of scales while keeping the computational requirement at an acceptable level. The outer LES resolves only the large turbulent structures, whereas the inner LES is dedicated to the small ones. The two models are coupled via the boundaries of the inner LES. A blending procedure acting in the vicinity of the coupled boundaries in the inner LES avoids discontinuities in the nested fields and smoothen the transition from the coarse-grained to the fine-grained fields.

Compared to a reference LES, the inner model of a nested-LES is able to reproduce the mean flow and higher statistics with great accuracy for a fraction of its computational time. The blending procedure smoothen the transition from the inner to the outer domain, where the fine-grained eddies of the LES are transformed to match the coarse-grained eddies imposed at the nested boundary. This feature is particularly useful in complex terrain or urban environment, where it is challenging to exactly define inlet and outlet boundaries. The blending distance and the relaxation time are the control parameters
Conclusions and Outlooks

of the blending procedure. The former defines the area affected by the blending inside the inner LES and the latter controls the strength of the blending. The optimal relaxation time is found to be correlated with the integral timescale.

A wind tunnel experiment has been conducted in order to mimic multiscale interactions in order to validate the nesting procedure. The Convective Boundary Layer (CBL) generated from a finite area heated plate, with or without wall mounted cubes, has been measured. Five cases were considered: a neutral case and four CBL cases with $\Delta T = 40, 60, 80$ and $100$ K. In the configuration without cubes, the buoyancy mostly affects the vertical turbulent fluxes $\langle u'_3 u'_3 \rangle$. The peak value of $\langle u'_3 u'_3 \rangle$ increases by a factor four in the most buoyant case and is shifted higher up in the boundary layer compared to the neutral case. The results of cases $\Delta T = 40 \& 60$ K, and $80 \& 100$ K show a clustering effect in the mean velocity, and the Reynolds stress components $\langle u'_1 u'_1 \rangle$ and $\langle u'_1 u'_3 \rangle$. In the configuration with cubes, a high level of Reynolds stresses is generated downstream each cube, especially in the shear layer. The buoyancy increases the Reynolds stresses by 20% to 50% in the cubes wake compared to the neutral case.

A LES of the configuration without cubes reproduces with good accuracy (within 5%) the mean velocity, mean temperature and Reynolds stresses. The effect of buoyancy are under-estimated most likely due to the grid resolution in the vertical direction and the turbulence model. A nested simulation is used to compute the configuration with cubes. The inner domain is able to reproduce the small turbulent structure around the cubes under the influence of the large buoyant structures modeled only in the outer domain. The mean and the higher order statistics match the measured data with good accuracy, with an error lower than 5% in most regions. As for the LES without cubes, the grid resolution in the vertical direction and the sgs-model can be improved for the buoyant cases.

The nesting procedure is finally applied to a real case. The flow around the ETHZ campus of Hönggerberg is resolved by an inner domain, whereas an outer domain resolve the entire ABL over several kilometers of terrain surrounding the campus. Both CBL and Neutral Boundary Layer (NBL) are simulated. The inflow of the outer domain is generated by a synthetic inflow generator which uses the flow statistics and lengthscales from two precursors LES of a CBL and a
The nested simulation is able to produce high quality results within the campus only for a fraction of the computational time required by a standard LES. The buildings in the inner domain generate a large roughness layer, which develops several hundreds of meters downstream the campus. Such roughness layer and far-field effect are not predicted by the wall-model of the outer LES.

7.2 Contributions to the Research Field

The nesting procedure proposed in this thesis fills the gap between highly resolved mesoscale Numerical Weather Prediction (NWP) with an horizontal resolution of 0.5 km and wind engineering simulations with wall cell of 50 cm in size. The outer domain of a nested-LES can simulate terrains with horizontal extent from $3 \text{ km} \times 3 \text{ km}$ to $10 \text{ km} \times 10 \text{ km}$ with a grid resolution of 10 m to 20 m near the ground. The inner domain can resolve the buildings with grid size down to 50 cm. The inner LES is connected to the outer LES through the coupled boundaries. In the vicinity of those boundaries, a blending procedure is applied to avoid inconsistency between the inner and the outer field in case of complex inlet-outlet flow. A synthetic turbulent inflow generator is proposed to drive the outer domain. The flow statistics from a precursor LES or from a 0.5 km mesoscale model can be used to feed the inflow generator. For the second solution, some approximations have to be made on the length scales and the anisotropy of turbulence (mesoscale NWP’s use isotropic turbulence models in general), but it allows to bridge all the scales together.

The nesting procedure has been validated with a reference simulation and a wind tunnel experiment. The comparison of the simulations with the measurements have shown that LES can predict CBL with good accuracy, but the effect of buoyancy should be more carefully treated. It is expected that the grid refinement in the vertical direction and a sgs-model with buoyancy correction can further improve the reliability of such simulations.

In a real full size configuration, it has been shown that the quality of the inner LES results strongly depends on the accuracy of the flow field in of the outer domain. The outer domain simulation has to be able to reproduce the effects of the parametrized roughness elements.
CONCLUSIONS AND OUTLOOKS

with a reasonable level of accuracy. As shown in the last chapter of this thesis, the roughness layer can extend downstream several times the characteristic size of the roughness elements.

7.3 OUTLOOKS AND PERSPECTIVES

A one-way downscale nested-LES opens interesting perspectives toward the resolution of multiscale interaction between the local weather and the flow through urbanized area. However, the presented method is open for further improvements:

- In a nested-LES, the inner domain resolves the roughness elements that are normally parametrized in the outer domain. Nevertheless, the outer domain should provide good approximation of the flow generated by the parametrized elements (i.e. the roughness elements). Actual wall-models for LES are designed to reproduce the effects of the roughness layer on the outer layer, not the roughness layer itself. Better wall-models need to be developed to specifically reproduce the drag and the blockage of the buildings.

- An urbanized area is not only characterized by its roughness. It can exchange heat, moisture and pollutants with the upper part of the ABL. Unlike the roughness, those fluxes vary during the day (solar irradiation, vegetation) and are influenced by the weather condition (humidity, rain, snow cover). Advanced LES wall-models should take into account those variations to correctly parametrize the roughness layer.

- The inner LES is able to generate finer turbulent structures due to its fine-grained grid. Those new structure take a certain distance to develop. If the nesting ratio is important, those new eddies can be triggered by adding synthetic turbulence at the coupled boundaries or in the blending zone. Existing synthetic inflow generator are designed to reproduce the full turbulent spectrum from the flow statistics. In this case, the outer domain is already turbulent, therefore only the missing small scale should be seeded at the coupled boundaries.
Two-way nesting is certainly the next major improvement after the one-way nesting presented in this thesis. The downsampling part is similar to the nesting procedure presented in this thesis. The upsampling part is performed by enforcing the results of the inner domain in the outer domain, at each timestep of the outer LES. Nevertheless, the upsampling presents several challenges:

- For the downsampling operation, the timestep $\Delta t^L_i$ and $\Delta t^L_{i+1}$ of the outer LES are used to compute the sub-timestep $\Delta t^S_i$ of the inner LES. In a two-way nesting, the inner solution at $\Delta t^S_{i+1}$ does not exist when the outer fields are computed at time $\Delta t^L_{i+1}$. Therefore a problem of simultaneity appears. It can be tackled by predicting the outer solution at timestep $\Delta t^L_{i+1}$ crudely before entering the inner loop (prediction step). After the inner loop is done, the data of the inner domain can be enforced in the outer domain, which can be finally accurately solved (correction step). The prediction-correction procedure proposed here is very similar to a PISO algorithm, which can be used as basis to achieve a two-way nesting.

- the upsampling operation is equivalent to a spatial low-pass filtering. Such filtering can break the conservation properties (mass, momentum and energy) of the flow. This problem can be solved by using interpolation methods which conserve mass, momentum and energy, or by using the property of a PISO algorithm, which corrects the predicted flow to enforce continuity.

- The inner fields have to be imposed in the outer ones during the upsampling operation. It can be done with an implicit blending term similar to the one proposed for the downsampling nesting procedure. The blending parameters should be chosen carefully to properly enforce the flow.

LES still remains a relatively costly simulation method compared to Reynolds Average Navier Stokes (RANS). Nevertheless, there are only a few further developments required to make LES a common research tool and a generally accepted operation tool for microscale prediction, in particular efficient wall-models and easy-to-use synthetic inflow generator. Efficient wall-models with accurate modeling of the roughness layer are needed in the outer domain of a nested-LES. Mesoscale
**Conclusions and Outlooks**

NWP models compute only the flow statistics (mean and Turbulent Kinetic Energy (TKE)), whereas the outer domain of a nested-LES needs time-dependent turbulent data at the inlet. Therefore a synthetic inflow generator can be used to bridge mesoscale NWP models with nested-LES models. The integration of those three scales (meso, micro, and urban) in an integrated numerical tool should allow the simulation of complex effects such as the Urban Heat Island (UHI), urban cooling by sea breeze and smog flushing. Those effects are influenced by the ABL stability, the buoyancy and the mechanical roughness which are studied in detail in this thesis. Nevertheless several other models need to be included to have a complete picture. For example, direct solar radiation, long wave radiation between buildings and vegetation have a large impact on the UHI. Among the different models available, LES still remains the most demanding in term of computational time (several days on a small cluster). Nevertheless, the quality of prediction it provides compared to faster but simpler flow models justifies the additional cost.


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186


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