

Analysis and modeling of small-scale turbulence

Emmanuel O. Akinlabi



UNIVERSITY
OF WARSAW

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Professor dr. hab. Szymon P. Malinowski
Dr. inż. Marta Waławczyk

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This thesis is dedicated to
my parents
James and Victoria Akinlabi

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Abstract

The analysis and modelling of small-scale turbulence in the atmosphere play a significant role in improving our understanding of cloud processes, thereby contributing to the development of better parameterization of climate models. Advancement in our understanding of turbulence can be fueled from a more in-depth study of small-scale turbulence, which is the subject of this thesis. Within this thesis, small scales are understood as turbulent structures affected by viscosity as well as scales from the high-wavenumber part of the inertial range which are of $\mathcal{O}(0.1m - 1m)$ typically neglected in numerical simulations of atmospheric turbulence.

This work is divided into two parts. In the first part, various approaches to estimate the turbulence kinetic energy (TKE) dissipation rate ϵ , from one-dimensional (1D) intersections that resemble experimental series, are tested using direct numerical simulation (DNS) of the stratocumulus cloud-top mixing layer and free convective boundary layer. Results of these estimates are compared with “true” DNS values of ϵ in buoyant and inhomogeneous atmospheric flows. This research focuses on recently proposed methods of the TKE dissipation-rate retrievals based on signal’s zero crossings and on recovering the missing part of the spectrum. The methods are tested on fully resolved turbulence fields and compared to standard retrievals from power spectra and structure functions. Anisotropy of turbulence due to buoyancy is shown to influence retrievals based on the vertical velocity component. TKE dissipation-rate estimates from the number of crossings correspond well to spectral estimates. As far as the recovery of the missing part of the spectrum is concerned, different models for the dissipation spectra was investigated, and the best one is chosen for further study. Results were improved when the Taylors’ microscale was used in the iterative method, instead of the Liepmann scale based on the number of signal’s zero crossings. This also allowed for the characterization of external intermittency by the Taylor-to-Liepmann scale ratio. It

was shown that the new methods of TKE dissipation-rate retrieval from 1D series provide a valuable complement to standard approaches.

The second part of this study addresses the reconstruction of sub-grid scales in large eddy simulation (LES) of turbulent flows in stratocumulus cloud-top. The approach is based on the fractality assumption of the turbulent velocity field. The fractal model reconstructs sub-grid velocity fields from known filtered values on LES grid, using fractal interpolation, proposed by Scotti and Meneveau [Physica D 127, 198–232 1999]. The characteristics of the reconstructed signal depend on the stretching parameter d , which is related to the fractal dimension of the signal. In many previous studies, the stretching parameter values were assumed to be constant in space and time. To improve the fractal interpolation approach, the stretching parameter variability is accounted for. The local stretching parameter is calculated from DNS data with an algorithm proposed by Mazel and Hayes [IEEE Trans. Signal Process 40(7), 1724–1734, 1992], and its probability density function (PDF) is determined. It is found that the PDFs of d have a universal form when the velocity field is filtered to wave-numbers within the inertial range. The inertial-range PDFs of d in DNS and LES of stratocumulus cloud-top and experimental airborne data from physics of stratocumulus top (POST) research campaign were compared in order to investigate its Reynolds number (Re) dependence. Next, fractal reconstruction of the subgrid velocity is performed and energy spectra and statistics of velocity increments are compared with DNS data. It is assumed that the stretching parameter d is a random variable with the prescribed PDF. Moreover, the autocorrelation of d in time is examined. It was discovered that d decorrelates with the characteristic timescale of the order of the Kolmogorov’s time scale and hence can be chosen randomly after each time step in LES. This follows from the fact that the time steps used in LES are typically considerably larger than Kolmogorov’s timescale. The implemented fractal model gives good agreement with the DNS and physics of stratocumulus cloud (POST) airborne data in terms of their spectra and PDFs of velocity increments. The error in mass conservation is smaller compared to the use of constant values of d . In conclusion, possible applications of the fractal model were addressed. A priori LES test shows that the fractal model can reconstruct the resolved stresses and residual kinetic energy. Also, based on the preliminary test,

the fractal model can improve LES velocity fields used in the Lagrangian tracking of droplets for the simulation of cloud microphysics.

Both parts of the thesis are based on the assumptions of scale self-similarity of Kolmogorov and local isotropy, which may not be satisfied in real atmospheric conditions. Since the standard methods for TKE dissipation rate retrieval are derived from these assumptions, the level of discrepancy is investigated by comparing the actual value of ϵ from DNS with estimates from these methods. Also, in the case of the modelling of small (sub-grid) scales, the improved fractal model relies on scale-similarity. Range of scales, in which this assumption is sufficiently satisfied (i.e. inertial range scales) is reconstructed. Statistical tools from the Kolmogorov's similarity hypotheses is used to assess the performance of the improved fractal model.

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Chapter 1

Introduction

Turbulent motions can be seen all around our world. H. Tennekes defines turbulence as “*the chaos that arises in fluids because of the innumerable instabilities associated with vortex stretching*” [142]. He and J. L. Lumley also define it in their book called “*A first course to turbulence*” through its characteristics: randomness, non-linearity effects, three-dimensional fluctuating vorticity, dissipating, enhance mixing and continuum [139]. Turbulence displays spatial and temporal structures over a wide range of scales. It has been long studied by both engineers and physicists such as O. Reynolds, A. N. Kolmogorov, W. K. Heisenberg, G. I. Taylor, L. Prandtl, T. von Karman etc. Most fluids in nature or engineering are turbulent unless it has low Reynolds or very stable stratification (more dense fluid below less dense fluid). Understanding turbulence is essential in many scientific disciplines such as in engineering (car engines, plane turbines), medicine (airflow in the lungs), financial markets, atmospheric and oceanic dynamics etc. Despite its importance and the long history of work done, a complete theory on turbulence is non-existent.

Atmospheric turbulence is a special form of turbulence caused by wind shear, buoyancy, surface roughness and convection, which can be severely intense. It is the key physical mechanism that is behind the occurrence of many atmospheric phenomena such as thunderstorms and the formation of rain, cyclones (see figure 1.1) etc. Turbulence in the atmosphere is the mechanism by which heat and moisture from the earth’s surface, as well as momentum, are mixed within the atmosphere. Other substances such as aerosols or pollutants are distributed both vertically and horizontally by turbulence.

The complexity observed in atmospheric turbulence is caused by its non-linear interacting nature. An interaction exists between different meteorological variables such as temperature, wind velocity, humidity etc. and a wide range of scales from large synoptic structures $\mathcal{O}(1000km)$ to the smallest dissipative eddies $\mathcal{O}(1cm - 1mm)$.

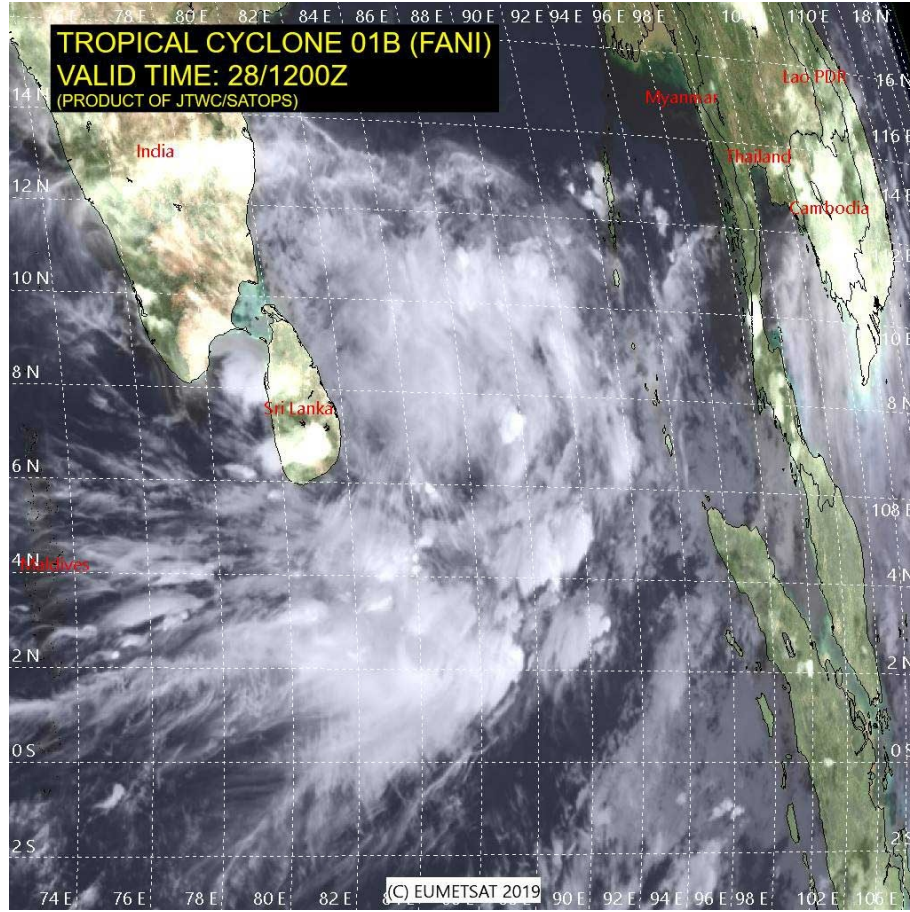


Figure 1.1: Tropical Cyclone Fani, formed over the Bay of Bengal, is moving towards the Andhra coast in India. Courtesy of EUMETSAT 2019

Typical Reynolds number $Re = \frac{UL}{\nu}$ of atmospheric flows is of the order $\mathcal{O}(10^9)$ where U is the characteristic velocity scale, L is the characteristic lengthscale and ν is the viscosity. All these scales play a role in weather prediction and other atmospheric events. The largest scales carry the memory of the physical system in which the flow is embedded while the small scales are somewhat “universal” or “quasi-universal” but can be highly intermittent.

Several attempts have been made to understand small-scale turbulence in the atmosphere due to its significant effect on numerous phenomena of practical interest. For example, collision rate, preferential concentration and average settling velocity of water droplets in clouds and precipitation are influenced by small scale motions [15, 67, 91, 109, 137, 155]. Moreover, a deeper understanding of small scale turbulence can advance the development of theories needed to explain turbulence. The classical theory of turbulence developed by Kolmogorov postulates that at sufficiently large Reynolds numbers, all symmetries of the Navier-Stokes equations are restored in a

statistical sense. However, the analysis of experimental data shows that this hypothesis is not valid for the scaling symmetries, which are broken at small scales due to intermittency [142]. According to the Kolmogorov’s first similarity hypothesis, small scales are statistically independent of the large scales at large Reynolds number, and their statistics can be described by the turbulence kinetic energy dissipation rate ϵ and the kinematic viscosity of the fluid ν . In the context of this thesis, the analysis and modelling of small-scale turbulence could improve our understanding of cloud processes and as a result, could possibly contribute to the improvement of numerical models.

The region of the atmosphere above the earth’s surface in which significant fluxes of most meteorological variables are transported by turbulent motions is called the atmospheric boundary layer. Example of this boundary layer is the free convective boundary layer, which is the region of the atmosphere affected by the heating of the earth’s surface by the sun. It is formed above the ground during the daytime when the atmosphere is unstable due to buoyancy forces. In the upper part of the atmospheric boundary layer, low-level clouds can be formed. An example is the stratocumulus-topped boundary layer, which is a well-mixed turbulent region of the troposphere in which clusters of stratocumulus clouds reside below the thermal inversion. They reflect to space a high percentage of incoming solar radiation, which helps to cool the earth’s surface. These boundary layers will be used in this thesis as test cases in the analysis and modelling of small scale atmospheric turbulence.

In this thesis, two simulation approaches to predict the evolution of turbulent flows will be addressed. In the numerical simulations, the Navier-Stokes equations are solved to determine $\mathbf{u}(\mathbf{x}, t)$ for one realization of the flow. The two approaches are direct numerical simulation (DNS) and large-eddy simulation (LES) [104]. In DNS, all length scales and timescales can be resolved when solving the Navier-Stokes equations for $\mathbf{u}(\mathbf{x}, t)$ with appropriate initial and boundary conditions. To resolve all scales, DNS requires huge computational resources and because the computational cost increases as Re^3 , this approach is confined to flows with low-to-moderate Reynolds numbers. Large-eddy simulation is used as a compromise to DNS to resolve the large scales features of the flow while sub-grid (unresolved) scales are modelled. These two approaches should be used together to understand better diverse phenomena in atmospheric boundary layer flows [87].

1.1 Aim of the thesis

This work focuses on the analysis and numerical reconstruction of small-scale turbulence in the atmosphere. An important quantity, which plays a crucial role in the study of small scales in turbulence, is the turbulence kinetic energy (TKE) dissipation rate ϵ [133]. First, the comparison of different methods for retrieving ϵ from atmospheric measurements will be carried out. The methods will be applied to investigate 1-D intersection of DNS velocity field of stratocumulus cloud top [119] and convective boundary layer [89]. Two common approaches used for retrieving ϵ are power spectral density and second-order structure function. Other methods based on zero crossings and recovering the missing part of the spectrum were introduced recently [144]. Moreover, the present work investigates how the presence of anisotropy (due to buoyancy and external intermittency) affects the various retrieval techniques of ϵ in the atmospheric configurations.

Second, the modelling of small-scales in atmospheric turbulence is investigated. Large-eddy simulations of atmospheric flows are usually computationally expensive because of the large range of scales required. For example, the boundary layer depth is of the order of few kilometres, the inversion region is of the order of few metres, and several kilometres is needed to include the largest eddies [82, 99]. As a result, most simulations are done at resolutions too coarse to resolve important processes [26]. The contribution of the unresolved (sub-grid) structures must be accounted for and this issue is considered as a major challenge in turbulence study. Small eddy structures from the inertial-range scales will be modelled using fractal interpolation technique (FIT). FIT is an iterative affine mapping procedure to construct the synthetic (unknown) small-scale eddies of the velocity field $\mathbf{u}(\mathbf{x}, t)$ from the knowledge of a filtered or coarse-grained field $\tilde{\mathbf{u}}(\mathbf{x}, t)$. Properties of the constructed sub-grid velocity depend on the stretching parameter d , which is related to the fractal dimension of the signal. Previous studies assume constant values of d in space and time. In this study, the spatial variability of d will be accounted for. Self-similarity of the PDF of d across different scales will be examined. This can be used to develop an improved FIT model for the reconstruction of small-scales in large-eddy simulations of atmospheric turbulence. The improved FIT model will be used to reconstruct sub-grid stresses, which can be used as a closure model for LES of atmospheric boundary layer flows. Also, the resolution of LES velocity field for the simulation of cloud microphysics will be improved.

Both parts of this thesis rely on Kolmogorov’s similarity hypotheses and the local isotropy assumption, which may not be satisfied in real atmospheric conditions. Statistical tools such as second- and third-order structure functions and power spectral density are derived from these hypotheses, which will be used to investigate the level of discrepancy by comparing the actual value of ϵ from DNS with estimates from these methods. Also, in the case of FIT, the major assumption is scale-similarity. The range of scales in which this assumption is sufficiently satisfied, which is the inertial-range scales, will be reconstructed. Statistical tools from Kolmogorov’s similarity hypotheses will be used to assess the performance of the FIT sub-grid model.

1.2 Thesis Overview

This thesis covers the results already published in Akinlabi et al. [*J. Atmos. Sci.*, **76(5)** 1471–1488, 2019], Akinlabi et al. [*Progress in Turbulence VIII. iTi 2018. Springer Proceedings in Physics*, vol 226. Springer, Cham] and Akinlabi et al. [*Flow, Turbul. Combust.*, **103(2)** 293–322, 2019]. The published papers were written together with my thesis advisors as coauthors. I did all the analysis and code development with the help of my thesis advisors. The last coauthor - Professor J-P Mellado (Max Planck Institute for Meteorology, Hamburg, Germany) provides both DNS dataset of stratocumulus-topped boundary layer and free convective boundary layer used in this thesis. I have rewritten and expanded the relevant parts of these published papers to account for the formal PhD thesis regulations. The application of the fractal subgrid model presented in chapter 9 was done recently (unpublished).

As a new contribution, the first part of the thesis investigates how the presence of anisotropy due to buoyancy and external intermittency affects the various retrieval techniques of ϵ in the atmospheric configurations including the new ones based on the number of crossings. Since direct numerical simulation (DNS) allows to verify the assumptions, I investigate the ϵ -estimation of these approaches and compare with the actual ϵ value from DNS of stratified atmospheric flows for two essentially different flow cases - stratocumulus cloud top and free convective boundary layer. In spite of the inhomogeneity and physical complexity of the flow, the calculated ϵ profiles generally agree with DNS values within a certain degree of accuracy. The observed deviations follow from the physical complexity of the flow and low-Re number of DNS as compared to real atmospheric conditions. This latter issue makes the spectral retrieval methods difficult due to the relatively short inertial range. Additional sources of error are the deviations of the Taylor-to-Liepmann microscale ratio from unity

as the assumption $\lambda_n/\Lambda \approx 1$ lies behind the number of crossing method [130]. I investigate an alternative form of the iterative method of Waławczyk et al (2017) [144] so as to remove these errors. I also study different forms of the model spectra in the iterative method. I show that λ_n/Λ can be used as a measure of external intermittency.

In the second part of the thesis, the modelling of small-scale turbulence in LES of the stratocumulus-topped boundary layer is studied. First, the investigation of the local values of d shows that it varies randomly both in space and time [5, 6, 118]. Then, the PDFs of d calculated from DNS data of stratocumulus-topped boundary layer, LES data in the same flow configuration and airborne dataset from the physics of stratocumulus (POST) campaign are compared. It is observed that independent of the Reynolds number of the flow considered, the PDFs of d collapse into one curve if the 1D intersection of the velocity fields were low-pass filtered to wave-numbers in the inertial-range. This finding is a new contribution of this thesis. Based on this, the new idea proposed here is to use random values of d , chosen from its PDF to reconstruct inertial-range (sub-grid) scales in LES. The autocorrelation function of d in time is examined. It is found that d decorrelates with the characteristic time-scale of the smallest eddies and hence can be chosen randomly after each time step in LES where time steps are considerably larger. I compare the performance of the new FIT approach with FITs with constant values of d . The energy spectra of the new FIT approach follow $-5/3$ Kolmogorov scaling more closely than in previous studies and have no spurious modulations. Also, the PDFs of velocity increments reproduce correctly the non-Gaussian, stretched-exponential tails when the improved FIT with random values of d is used. For LES application, the improved FIT is extended to three dimensions. Mass conservation, which can be violated when using FIT, is addressed. It is shown that after two reconstruction steps, the error in mass conservation of the reconstructed field is of the same order of magnitude as the error of filtered LES without reconstruction. I address the cost of LES with FIT and observe that the CPU time of LES with FIT (three reconstruction steps) is the same order of magnitude as the CPU time of LES. In the final part of this thesis, I work on the possible application of the improved fractal model. I show that the fractal model can be used to reconstruct the resolved stresses of a test filter and the residual kinetic energy in LES. Based on the preliminary test done, the new fractal model can be used to reconstruct subgrid scales for the LES velocity field used in the Lagrangian tracking of super-droplet in models for simulating cloud microphysics.

The dissertation is organized as follows. A review of the classical turbulence theory and the governing equations used in the numerical simulation of the atmospheric boundary layer is presented in chapter 2. It begins with a brief literature review, which includes the concept of energy cascade and Kolmogorov’s similarity hypotheses. It continues with a description of the two approximations (anelastic and Boussinesq) of the Navier-Stokes equation often used for simulating atmospheric motions. It concludes with a summary of the averaging and filtering operators that can be applied to the governing equations and the LES technique. Chapter 3 contains an introduction to the first part of this thesis. It explains the concept of turbulence kinetic energy dissipation rate ϵ and outlines the various retrieval methods used to estimate ϵ from 1D velocity time series. In chapter 4, the two DNS datasets used in this thesis are briefly described. The analysis of ϵ with different retrieval techniques is discussed in chapter 5. It starts with the analysis of ϵ in DNS datasets of stratocumulus cloud-top and free convective boundary layer with methods related to the inertial-range scaling. Next, it continues with error analyses of these methods and investigates the influence of finite sampling on ϵ estimates. It concludes with the estimation of ϵ using direct and iterative methods and shows that λ_n/Λ can be used as a measure of external intermittency. Chapter 6 introduces the second part of the thesis. It presents the motivation and a brief overview. Description of the fractal subgrid-scale model is presented in chapter 7. It starts with a short description of FIT and describes the Mazel and Hayes [83] algorithm to calculate local values of d . Next, a brief description of the POST airborne campaign and LES of stratocumulus topped boundary layer is presented. The comparison between the PDFs of d computed from DNS, LES and POST datasets is shown. The chapter concludes with evaluating the autocorrelation function of d in time. In chapter 8, the new FIT with random values of d is compared with FITs with constant value of d . It shows the application of the new FIT approach to 3D LES velocity fields and addresses the deviation of FIT velocity fields from mass conservation. It ends with an investigation on the computational cost required by FIT. Chapter 9 outlines possible applications for the new FIT model. It explains how the resolved stresses for a test filter and residual kinetic energy can be reproduced with the FIT. It also explores the reconstruction of inertial-range subgrid scales for the Lagrangian tracking of super-droplets in LES velocity field.

Chapter 2

Theoretical Background

In this chapter, theoretical background for the study of turbulence is introduced. The starting point is the discussion about the turbulent energy cascade of Richardson (1922) [114] and the Kolmogorov's similarity hypotheses [64]. This chapter highlights the governing equations (anelastic and Boussinesq approximations) used for the direct numerical simulation of the atmospheric boundary layer. To simplify these equations, an averaging and filtering operator used to derive the Reynolds equations and large-eddy simulation (LES) respectively are presented. It concludes with an outline of the governing equations used for the LES of atmospheric boundary layer.

2.1 Energy cascade and Kolmogorov's similarity hypotheses

The energy cascade idea, introduced by Richardson (1922) [114], is a milestone in classical turbulence theory. This idea describes turbulence as a composition of eddies (or turbulent motions) of different sizes and continuously evolving by interacting with each other [22]. Eddies are characterized by size l , a characteristic velocity $u(l)$ and time scale $\tau(l) = l/u(l)$. Turbulence eddies in the largest size range (characterized by length-scale $l = l_0$) are unstable. They break up, transferring their kinetic energy into smaller and smaller eddies until the vortices are sufficiently small (with size $l \ll l_0$), stable and their kinetic energy is dissipated by viscous effects. This idea assumes that the rate of kinetic energy dissipation ϵ is determined by the transfer rate of energy from the largest eddies, which are of the order of the root-mean-square of turbulence intensity [104, 142].

$$u' = \left(\frac{2K_e}{3} \right)^{1/2} \quad (2.1)$$

where $K_e = \langle u_i u_i \rangle / 2$ is the turbulence kinetic energy.

Kolmogorov's hypotheses [64] were developed from the idea of the energy cascade. Kolmogorov argued that the anisotropy of large scales are lost as energy is transferred to successively smaller eddies. This is summarized in the first hypothesis, which is about the isotropy of small scales (or eddies). It states that:

Kolmogorov's hypothesis of local isotropy. *“At sufficiently high Reynolds numbers, the small-scale turbulent motions ($l \ll l_0$) are statistically isotropic” [64, 142].*

Kolmogorov's first similarity hypothesis. *“At sufficiently high Reynolds number, the statistics of small scale motions have a universal form that is uniquely determined by viscosity ν and ϵ ” [104].*

From the first similarity hypothesis, the unique Kolmogorov's length, velocity and time scales can be formed

$$\begin{aligned}\eta &\equiv (\nu^3/\epsilon)^{1/4} \\ u_\eta &\equiv (\epsilon\nu)^{1/4} \\ \tau_\eta &\equiv (\nu/\epsilon)^{1/2}\end{aligned}\tag{2.2}$$

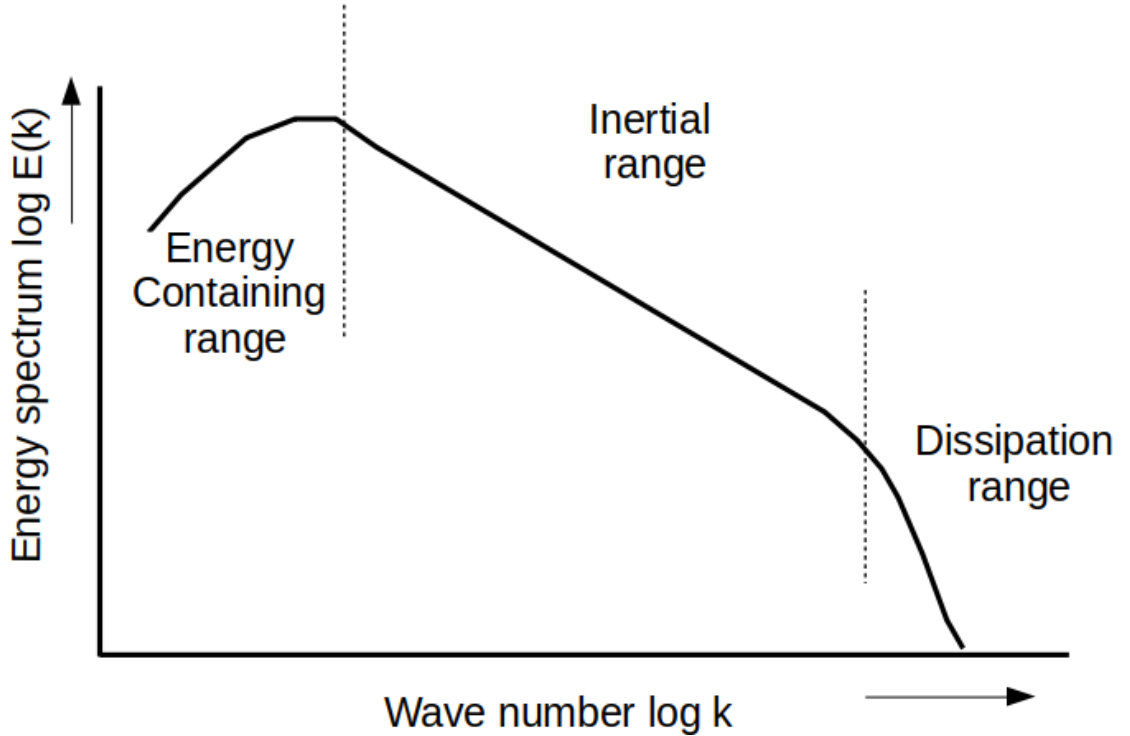


Figure 2.1: Kolmogorov's energy spectrum $E(k)$ as a function of wave number k

The ratio of characteristic length of the smallest scales of motion to the largest one (i.e. η/l_0) decreases with the increase in Reynolds number. Scales of motion in turbulence can be divided into three length-scale ranges. The energy-containing range has the bulk of the kinetic energy, which are contained in the larger eddies. The range of turbulent scales that are influenced by viscosity and responsible for all energy dissipation are called the dissipation range while the inertial (sub)range are only determined by inertia effects. The existence of the inertial-range scales forms the basis of the second similarity hypothesis, which states that:

Kolmogorov's second similarity hypothesis. *"At sufficiently high Reynolds number turbulent flows, there exist scales of motion (of size l) in the range $\eta \ll l \ll l_0$ such that their statistics are uniquely determined by ϵ and independent of ν " [104].*

In wavenumber k space, the energy contributed by scales with wavenumbers between k and $k+dk$ can be written as $E(k)dk$. The energy contained with a wavenumber range (k_i, k_{i+1}) is given as

$$K_e = \int_{k_i}^{k_{i+1}} E(k)dk \quad (2.3)$$

Within the inertial range, the energy $E(k)$ depends only on ϵ . Hence, the energy should scale as

$$E(k) \sim \epsilon^{2/3} k^{-5/3}. \quad (2.4)$$

This is called the Kolmogorov's energy spectrum or $-5/3$ scaling law. Figure 2.1 shows the Kolmogorov's energy spectrum $E(k)$ as a function of wave number k .

Most of the methods for retrieving ϵ that will be discussed in chapter 3 are based on the Kolmogorov's similarity hypotheses. In chapter 7, the assumption of scale similarity in inertial-range scales is used to reconstruct sub-grid scales of motion using fractal interpolation technique.

2.2 Governing equations for simulating atmospheric turbulence

The basic evolution equations for the simulation of atmospheric motion are based on the anelastic [96, 98] or the Boussinesq approximation [141] of the Navier-Stokes equations. These approximations are discussed below.

2.2.1 Boussinesq approximation

The Boussinesq approximation is used in buoyancy-driven flows such as in free convective boundary layer, oceanic circulation, atmospheric fronts etc. It assumes that the density variations are negligible and only appear with the term containing gravitational acceleration. Sound waves are completely neglected when using this approximation since sound waves propagate via density variation [141]. The Boussinesq equations can be written in the form [89]:

$$\nabla \cdot \mathbf{u} = 0, \quad (2.5)$$

$$\frac{D\mathbf{u}}{Dt} = -\nabla p + \nu \nabla^2 \mathbf{u} + b\hat{\mathbf{z}} \quad (2.6)$$

$$\frac{Db}{Dt} = \kappa \nabla^2 b \quad (2.7)$$

where $\mathbf{u}$ is the velocity field, p is a modified pressure divided by the constant reference density, ν is the kinematic viscosity, κ is the molecular diffusivity and b is the buoyancy. The buoyancy relates to the virtual potential temperature θ through

$$b = \frac{g(\theta - \theta_0)}{\theta_0}. \quad (2.8)$$

where θ_0 is the reference value obtained if the linear stratification of θ in the free atmosphere is extrapolated to the earth's surface. The reference buoyancy varies as $N^2 z$ where N^2 is a constant buoyancy gradient. The atmosphere can be in three configurations: a neutral stratification $N^2 = 0$, stable stratification $N^2 > 0$ or an unstable stratification $N^2 < 0$. This approximation is used in the DNS of free convective boundary layer discussed in section 4.2.2.

2.2.2 Anelastic approximation

The anelastic approximation is suitable for atmospheric boundary layer dynamics and deep moist convection applications [21, 96, 98, 111]. The anelastic equations remove sound waves, thereby reducing the computational cost that arises in explicit time integration of the fully compressible Navier-Stokes equations. This approximation is justified by the small Mach number of atmospheric dynamics [34, 111]. The anelastic approximation is based on linearizing pressure and density fluctuations around a

reference state of constant moist entropy. The reference state for the pressure $p_0(z)$ and density $\rho_0(z)$ are given by the hydrostatic balance,

$$\frac{\partial p_0}{\partial z} = -\rho_0 g. \quad (2.9)$$

The reference density ρ_0 is a function of the specific entropy s_0 , total water specific humidity $q_{t,0}$ and pressure p_0 .

Let consider a moist atmosphere (such as in the stratocumulus-top boundary layer [119]), which is an ideal mixture of dry air, water vapour and liquid water. Thermodynamic variables such as temperature can be assumed to be in equilibrium. Water that is not in equilibrium with the surrounding air can be treated separately. Thus, the total water specific humidity of the fluid can be defined as $q_t = q_v + q_l + q_i$ ($q_i = 0$ for warm clouds), where q_v, q_l and q_i are the water vapour, liquid and ice specific humidities of the water phases in local thermodynamic equilibrium [98]. By applying the Gibbs' phase rule, all thermodynamic-equilibrium variables can be estimated from the entropy s , total water specific humidity q_t and pressure $p = p_0 + p'$. As discussed in Pauluis (2008) [98], the anelastic equations require that the dynamic pressure perturbation p' can be neglected, and the thermodynamic error due to this approximation is small in most situation in the Earth atmosphere [69]. The anelastic equations used by Ref. [87] are in form

$$\nabla \cdot (\rho_0 \mathbf{u}) = 0, \quad (2.10)$$

$$\frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho_0} \nabla p' + b\hat{\mathbf{z}} - f(\mathbf{u} - \mathbf{u}_g) \times \hat{\mathbf{z}} + \nu \nabla^2 \mathbf{u} + \omega \partial_z \mathbf{u} + \Sigma, \quad (2.11)$$

$$\frac{Dh}{Dt} = \frac{1}{\rho_0} \nabla \cdot [\rho \kappa_h \nabla h - \rho \mathbf{j}_\mu (h_l - h) - \rho \mathbf{j}_r] + \omega \partial_z h, \quad (2.12)$$

$$\frac{Dq_t}{Dt} = \frac{1}{\rho_0} \nabla \cdot [\rho \kappa_v \nabla q_t - \rho \mathbf{j}_\mu (1 - q_t)] + \omega \partial_z q_t, \quad (2.13)$$

$$\frac{Dq_l}{Dt} = \frac{1}{\rho_0} \nabla \cdot [\rho \kappa_v \nabla q_l - \rho \mathbf{j}_\mu (1 - q_l)] + \omega \partial_z q_l + \frac{\rho}{\rho_0} \left(\frac{\partial q_l}{\partial t} \right)_{con}, \quad (2.14)$$

where $D/Dt = \partial/\partial t + \mathbf{u} \cdot \nabla$ is the material derivative, $\mathbf{u}$ is the velocity field, ω is the large scale subsidence velocity, $\rho \mathbf{j}_\mu$ is the liquid mass flux, $\rho \mathbf{j}_r$ is the radiative flux, $\frac{\rho}{\rho_0} \left(\frac{\partial q_l}{\partial t} \right)_{con}$ is the condensation rate, κ_h is the thermal diffusivity, κ_v is the diffusivity of water vapour in dry air, Σ is a momentum source, ν is the kinematic viscosity, f is the Coriolis parameter ($f = 0$ for DNS because the computational domain is too

small for the Coriolis force to be important), $\mathbf{u}_g$ is the large-scale geostrophic velocity and b is the buoyancy defined as

$$b = \frac{g(\rho - \rho_0(z))}{\rho_0(z)} \quad (2.15)$$

where g is the magnitude of acceleration due to gravity. The term $\omega \partial_z \Psi$ (where Ψ represents $\mathbf{u}$, h , q_t or q_l) is added to these equations to account for the effect of large turbulent eddies that are not represented in DNS of stratocumulus-top boundary layer [119]. The liquid water static energy h is defined as

$$h \equiv [c_d + q_t(c_v - c_d)]T - q_l L_v + gz \quad (2.16)$$

where the latent heat of vapourization L_v varies with the temperature as $L_v = L_{v,0} - (c_l - c_v)(T - T_0)$. The specific heat capacities at constant pressure of dry air, c_d , water vapour, c_v and liquid water, c_l are constant. Equations 2.13 and 2.14 are prognostic equations for the total water and liquid water specific humidities respectively. This anelastic approximation is used in the DNS of stratocumulus-top boundary layer discussed in section 4.2.1.

2.2.3 Averaging and filtering

In general, turbulent flows can be described as a random field since their velocity components at a point fluctuate with time in a random manner [104]. To describe turbulence, its averaged quantities, which are measurable in experiments can be used. Starting with the Navier-Stokes equation, it is possible to derive equations for the evolution of these averaged quantities (for example, Reynolds equation for the mean velocity field $\langle \mathbf{U}(\mathbf{x}, t) \rangle$). The ensemble average is defined for flows that can be repeated N times as

$$\langle \mathbf{U}(\mathbf{x}, t) \rangle_N \equiv \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N U^{(n)}(\mathbf{x}, t), \quad (2.17)$$

where $\mathbf{U}^{(n)}(\mathbf{x}, t)$ is the measurement on the n th realization. The ensemble average commutes with other linear operations such as integration and differentiation [152].

Other approximations for the ensemble average $\langle \mathbf{U}(\mathbf{x}, t) \rangle$ can be used in turbulent flow experiments and simulations [104, 152]. In statistically stationary flows, the time average over a time interval T is defined as [104]

$$\langle \mathbf{U}(\mathbf{x}, t) \rangle \approx \langle \mathbf{U}(\mathbf{x}, t) \rangle_T \equiv \frac{1}{T} \int_t^{t+T} U(\mathbf{x}, \tau) d\tau. \quad (2.18)$$

In homogeneous turbulence simulations, the ensemble average can be replaced by the spatial average over a cubic domain of sizes L_x in x -direction, L_y in y -direction and L_z in z -direction is defined as [104]

$$\langle \mathbf{U}(\mathbf{x}, t) \rangle \approx \langle \mathbf{U}(\mathbf{x}, t) \rangle_{x,y,z} \equiv \frac{1}{L_x L_y L_z} \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} \mathbf{U}(\mathbf{x}, t) dx dy dz \quad (2.19)$$

The evolution equations for the averaged quantities have significant limitations in describing flows found in nature (especially in the atmosphere) because these flows are (in most cases) unsteady and exhibit spatial and temporal structures in a range of scales. For a full description of turbulence, it would be best to solve the Navier-Stokes equations in its “pure” form without any approximations. This approach is performed in DNS. DNS imposes huge computational cost, which increases as Re^3 , because all length-scales and time-scales have to be resolved. As a result, this approach is only restricted to flows with moderate Reynolds number [104]. Most of the computational resources in DNS are consumed on resolving the smallest scales, whereas most of the energy is contained in the larger scales of motion. For this reason, it is necessary to apply a filtering operation on the solution $\mathbf{u}(\mathbf{x}, t)$ of the Navier-Stokes equations, decomposing it into its filtered (or resolved) component $\tilde{\mathbf{u}}(\mathbf{x}, t)$ and a residual (or sub-grid scale) component $\mathbf{u}'(\mathbf{x}, t)$. This filtering process makes the simulation of high Reynolds number flows possible. Leonard (1974) [72] define the filtering operation over the entire flow domain as

$$\tilde{\mathbf{u}}(\mathbf{x}, t) = \int G(\mathbf{r}, \mathbf{x}) \mathbf{u}(\mathbf{x} - \mathbf{r}, t) d\mathbf{r}, \quad (2.20)$$

where G satisfies the normalization condition

$$\int G(\mathbf{r}, \mathbf{x}) d\mathbf{r} = 1. \quad (2.21)$$

Any homogeneous filter function can be used to filter the Navier-Stokes equations. Examples are the spectral cut-off, top-hat and Gaussian filter functions [104, 152]. Evolution equation for the filtered component $\tilde{\mathbf{u}}(\mathbf{x}, t)$ is called the filtered Navier-Stokes equations. This filtered equations are solved in LES, which is discussed in section 2.3.

2.3 Large-eddy simulation

Applying a filtering operation (discussed in section 2.2.3) on the Navier-Stokes equation is the basis of LES, in which the larger turbulent scales of motion are directly

solved for, while the effects of smaller scales are represented with sub-grid scale models. Atmospheric applications motivated most of the early works on LES (e.g. see [73, 127]). An overview of the applications of LES were compiled by Galperin and Orszag (1993) [148]. One of the major usage of LES is in the study of atmospheric boundary layer (e.g. see [20, 81, 82, 122]).

In deriving the filtered form of the governing equations for atmospheric turbulence in anelastic approximation (equations 2.10 - 2.14) [96], the basic assumption is to decompose the thermodynamic state variables into its horizontally averaged quantity (denoted with a subscript “0”, which varies only in the z - direction) and the perturbation (indicated with “prime” as superscript). The humid equation of state is used in deriving the momentum equation [122]

$$p = \rho RT(1 + 0.61q_v), \quad (2.22)$$

where p is the pressure, R is the gas constant, ρ is the density and q_v is the mixing ratio of water vapour. The pressure is nondimensionalized with the reference pressure p_0 as

$$\pi = (p/p_0)^{R/c_p}, \quad (2.23)$$

where c_p is the specific heat of dry air at constant pressure. The potential temperature is defined as

$$\theta = \frac{T}{\pi}. \quad (2.24)$$

In LES of moist atmosphere such as in the stratocumulus-top boundary layer, the equation for potential temperature replaces the equation for static energy h in equation 2.12. The anelastic form of the Navier-Stokes equation reads [122]

$$\frac{\partial \rho_0 \tilde{u}_i}{\partial x_i} = 0, \quad (2.25)$$

$$\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial \tilde{u}_i \tilde{u}_j}{\partial x_j} = \theta_0 \frac{\partial \pi'}{\partial x_i} + \delta_{i3} \frac{g}{\theta_0} (\theta_v - \langle \theta_v \rangle) - \frac{\partial \tau_{ij}}{\partial x_j} + F_i, \quad (2.26)$$

$$\frac{\partial \tilde{\theta}}{\partial t} + \frac{\partial \tilde{u}_i \tilde{\theta}}{\partial x_i} = -\frac{\partial \sigma_{j\theta}}{\partial x_j} + \frac{L\theta_e}{c_p T_e} C + Q_{rad}, \quad (2.27)$$

$$\frac{\partial \tilde{q}_v}{\partial t} + \frac{\partial \tilde{u}_i \tilde{q}_v}{\partial x_i} = -\frac{\partial \sigma_{jq_v}}{\partial x_j} - C, \quad (2.28)$$

$$\frac{\partial \tilde{q}_c}{\partial t} + \frac{\partial \tilde{u}_i \tilde{q}_c}{\partial x_i} = -\frac{\partial \sigma_{jq_c}}{\partial x_j} + C, \quad (2.29)$$

where g is the gravitational acceleration, θ_v is the virtual potential temperature, L is the latent heat of condensation, c_p is specific heat at constant pressure, subscript e represents hydrostatically balanced environmental profile. $\tau_{ij}, \sigma_{j\theta}, \sigma_{jq_c}, \sigma_{jq_v}$ are sub-grid stresses of momentum, potential temperature, water vapour and liquid water mixing ratios respectively. Q_{rad} is the source due to radiative transfer, C is the condensation rate and F_i is the Coriolis force. For the full description of Q_{rad} , C and F_i , readers are referred to Ref. [66, 82, 99, 135]. Equations 2.25 - 2.29 were used in LES of stratocumulus-top boundary layer (discussed in section 7.3.2). The filtered form of the governing equations in Boussinesq approximation is similar to the anelastic form except that the density variation is negligible and appears only through the term with gravitational acceleration and the prognostic equations for q_v , q_l is absent since the approximation is applied to dry convective atmosphere. Readers are referred to Ref. [20] for details.

Part 1

Retrieving information of small-scale turbulence

Chapter 3

Estimating turbulence kinetic energy dissipation rate

This chapter introduces the concept of turbulence kinetic energy dissipation rate ϵ . It outlines the various retrieval methods used to estimate ϵ from 1D velocity time series.

Since the groundbreaking work of Kolmogorov [64], it is widely known that the quantity, which plays a crucial role in the study of small-scale turbulence is the turbulence kinetic energy (TKE) dissipation rate [133]. This quantity determines the amount of energy lost by the viscous forces when the energy of the eddies dissipates (at the molecular level) into heat. In statistically steady turbulence, the energy dissipation rate is equivalent to the energy transfer rate from large to small scales in the energy cascade with an assumption that the eddies break up successively through inertial forces until their size is of the same magnitude as the Kolmogorov length scale ($\eta \equiv (\nu^3/\epsilon)^{1/4}$). A robust estimation of ϵ is needed to formulate collision kernel model required to simulate cloud processes [16, 48, 60] (e.g. rain formation), perform Lagrangian trajectory analysis of passive scalars [101] or parameterize phenomenon in numerical models of different spatial and temporal scales. Numerical schemes that use such formulations range from pollution dispersion to weather and climate forecast models [38].

Numerous authors have estimated ϵ with experimental data in different context such as wake vortices [39], atmospheric boundary layers [42, 63, 78, 126], stratified flows in wind tunnel [38], jet flows [12], mixer [151], water vessel [138] etc. Others have used numerical simulation data to estimate ϵ in configurations such as homogeneous isotropic turbulence [132, 153], cylinder wake flow [71], turbulent channel flow [2] etc.

In the literature, several methods have been proposed to calculate ϵ from 1D velocity time series, using the local isotropy assumption. Two types of methods are

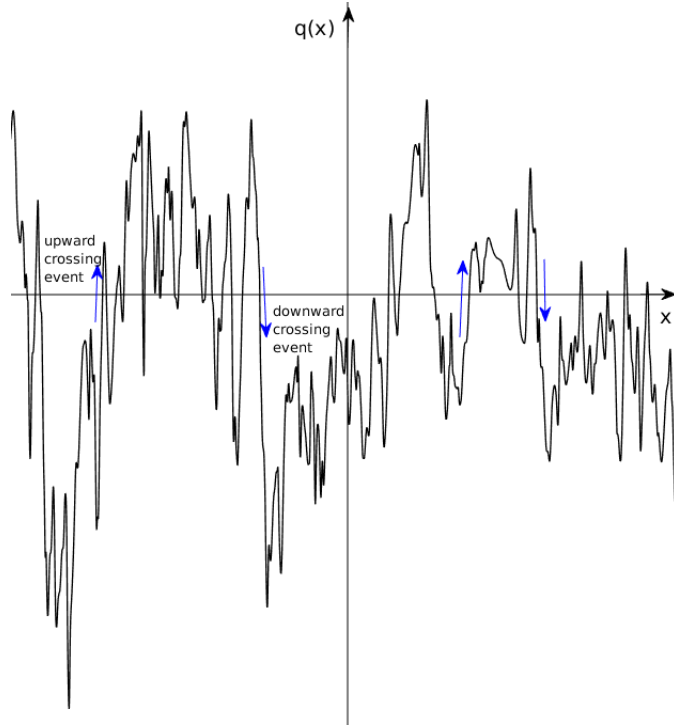


Figure 3.1: Description of zero-crossing approach

predominantly used: direct and indirect methods. In case of fully-resolved velocity signals, the direct methods, based on measuring the variance of velocity fluctuation gradients, can be applied. Alternatively, Sreenivasan et al. (1983) [130] proposed to use the zero-crossing approach, which requires counting the number of times N_L the velocity signal crosses the zero threshold per unit length, see figure 3.1. The so-called Liepmann scale defined as $\Lambda = 1/(\pi N_L)$ is assumed to be equal to the transverse Taylor’s microscale λ_n , which is used to calculate ϵ . The indirect methods are based on the inertial range scaling argument of $-5/3$ that follow from the Kolmogorov’s similarity hypotheses [10, 64] discussed in section 2.1. Such methods are commonly used in the analysis of low and moderate resolution velocity time series from in-situ airborne measurements [65, 124] or particle image velocimetry data [153]. The two common indirect methods are the power spectra density and structure functions.

All the above described indirect methods for ϵ retrieval are based on the Kolmogorov’s local isotropy assumption. This assumption may not always be fulfilled in real atmospheric conditions [29], which is influenced by buoyancy. The energy spectra of buoyancy-driven turbulence has been studied by several authors [23, 68, 74, 75, 145]. First, Bolgiano (1959) [23] and Obukhov (1959) [95] proposed that the energy spectrum should scale as $E(k) \sim k^{-11/5}$ in stably stratified flows (referred to as BO

scaling), where k is the wavenumber. Such scaling was later assumed to hold also in thermally-driven flows, however, a fine resolution simulation performed by Kumar et al. (2014) [68] revealed that turbulent convection exhibits Kolmogorov’s energy spectrum. This was also confirmed by Verma et al. (2017) [143] in their DNS study of Rayleigh-Benard Convection at $Pr \approx 1$. Regarding stably stratified turbulence, Verma et al. (2017) [143] argued that in case of comparable strengths of gravity and the nonlinear, convective term in the Navier-Stokes equations (in equation (2.11) or (2.6)), nearly isotropic turbulence with BO scaling is obtained. On the other hand, strong nonlinearity yields the hydrodynamic spectrum with the Kolmogorov scaling. Finally, strong gravity, as compared to the nonlinear term makes the flow similar to 2D hydrodynamic turbulence. Kimura and Herring (2012) [61] investigated homogeneous incompressible turbulence subjected to a range of degrees of stratification using pseudo-spectral DNS method. The authors argued that anisotropy is significant even in kinetic energy dissipation and that a single three-dimensional dissipation rate can not provide a universal Kolmogorov constant.

The physically complex atmospheric turbulence is not only inhomogeneous or buoyancy-driven but also includes the co-existence of laminar and turbulent regions called external intermittency [54, 140]. The volume fraction occupied by a turbulent signal is called the intermittency factor γ . For purely laminar signal $\gamma = 0$ and $\gamma = 1$ for purely turbulent flow.

3.1 Direct methods

In direct methods, the gradients of velocity are measured. The TKE dissipation rate is defined as (see e.g. [104])

$$\epsilon = 2\nu \langle s_{ij}s_{ij} \rangle, \quad \text{where} \quad s_{ij} = \frac{1}{2} \left(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right), \quad (3.1)$$

s_{ij} is the fluctuating strain rate tensor, $u'_i = u_i - \langle u_i \rangle$ denotes the i -th component of fluctuating velocity, $\langle \cdot \rangle$ is the ensemble average operator and ν is the kinematic viscosity of the fluid. The exact definition cannot be used to estimate ϵ in case only 1D intersections of turbulent velocity field are available from experiments. Additionally, the resolution of the measured signals can be deteriorated due to finite sampling frequency of a sensor, as well as measurement errors.

In the case a turbulent signal is resolved down to the smallest scales, the ”direct” relation between the TKE dissipation rate and the longitudinal, or transverse Taylor

microscale can be used

$$\epsilon_\lambda = 15\nu \frac{\langle u_l'^2 \rangle}{\lambda_n^2} = 30\nu \frac{\langle u_l'^2 \rangle}{\lambda_l^2}. \quad (3.2)$$

The longitudinal Taylor microscale equals

$$\lambda_l = \left[\frac{2\langle u_l'^2 \rangle}{\langle (\partial u_l' / \partial x)^2 \rangle} \right]^{1/2} \quad (3.3)$$

and transverse microscale is $\lambda_n = \lambda_l / \sqrt{2}$. In case of isotropy, ϵ_λ coincides with ϵ . The difference between ϵ and ϵ_λ is quantified. It will be shown later that the difference between these estimates are caused by the anisotropy introduced by buoyancy and shear forcings, and by external intermittency.

Other direct methods for calculating TKE dissipation rate based on number of zero-crossings was proposed by Sreenivasan et al. (1983) [130] and used by many authors, see e.g. [102, 103, 150, 154]. Zero-crossings method was first introduced by Rice (1945) [113] assuming that a stochastic process q and its derivative with respect to time $\partial q / \partial t$ have Gaussian statistics and are statistically independent. This method was derived from evaluating the number of times the signal crosses the level zero i.e. $q(t) = 0$ (see figure 3.1). Then, the square of the number of zero-crossings N per unit time is

$$N^2 = \frac{\langle (\partial q / \partial t)^2 \rangle}{\pi^2 \langle q^2 \rangle}. \quad (3.4)$$

Sreenivasan et al. (1983) [130] considered the Liepmann scale defined as

$$\Lambda = \frac{1}{\pi N_l}, \quad (3.5)$$

where N_l is a number of crossings of fluctuating velocity component u_l' per unit length, and using the formula (3.4) assumed that $\Lambda \approx \lambda_n = \lambda_l / \sqrt{2}$, hence

$$\frac{\lambda_n}{\Lambda} \approx 1. \quad (3.6)$$

For this, it was argued in Sreenivasan et al. (1983) [130] that Eq. (3.4) also holds for strongly non-Gaussian velocity signals (or for non-Gaussian derivative of the time series). This implies that strong departure from Gaussianity do not necessarily yield values appreciably different from unity for the ratio of λ_n / Λ .

One-dimensional longitudinal and transverse energy spectra E_{11} and E_{22} , respectively, are related to the energy spectrum function $E(k)$ by [104]

$$E_{11}(k_1) = \int_{k_1}^{\infty} \frac{E(k)}{k} \left(1 - \frac{k_1^2}{k^2} \right) dk, \quad E_{22}(k_1) = \frac{1}{2} \int_{k_1}^{\infty} \frac{E(k)}{k} \left(1 + \frac{k_1^2}{k^2} \right) dk. \quad (3.7)$$

where k_1 is the longitudinal component of the wavenumber vector $\mathbf{k}$. For a spatially varying signal, equation (3.4) can be written as

$$N_l = \frac{1}{\pi} k_c \quad (3.8)$$

where k_c is the characteristic wavenumber, which can be written as

$$k_c = \sqrt{\frac{\int_0^\infty k^2 E_{11} dk}{\int_0^\infty E_{11} dk}}. \quad (3.9)$$

Based on this result and Eq. (3.2), Sreenivasan et al. (1983) [130] proposed a formula for calculating ϵ , applicable to fully-resolved signals (measured down to the smallest dissipative eddies), which reads

$$\epsilon_{SR} = 15\pi^2 \nu \langle u_l'^2 \rangle N_l^2, \quad (3.10)$$

or for number of crossings N_n calculated from the time series of transverse velocity fluctuation component u_n'

$$\epsilon_{SR} = \frac{15}{2} \pi^2 \nu \langle u_n'^2 \rangle N_n^2. \quad (3.11)$$

The number of crossings is related to the energy spectra E_{11} by the formula

$$\pi^2 \langle u_l'^2 \rangle N_l^2 = \int_0^\infty k^2 E_{11} dk. \quad (3.12)$$

In case a signal is low-pass filtered, the number of zero-crossings per unit length depends on cut-off wavenumber.

3.2 Indirect methods

The indirect methods relate the small-scale phenomenon of dissipation with the inertial-range scales as predicted by the second Kolmogorov's hypothesis [64]. The two common indirect approaches use the inertial-range scaling form of the power spectra and structure functions. In the homogeneous and isotropic turbulence, the following energy spectrum is assumed [104]

$$E(k) = C \epsilon_{PS}^{2/3} k^{-5/3} f_L(kL) f_\eta(k\eta) \quad (3.13)$$

where $C \approx 1.5$ derived from experimental data, f_L and f_η are non-dimensional functions. The term ϵ_{PS} should be equal to the TKE dissipation rate ϵ if the second similarity hypothesis is satisfied.

Functions f_L and f_η specify the shape of the energy-spectrum in the energy-containing range and the dissipation range respectively. L is the length scale of large eddies and $\eta = (\nu^3/\epsilon)^{1/4}$ is the Kolmogorov length scale, which is connected with the dissipative scales. The function f_η tends to unity for small $k\eta$ while f_L tends to unity for large kL , such that in the inertial range, the formula $E(k) = C\epsilon_{PS}^{2/3}k^{-5/3}$ is recovered. Pope (2000) [104] proposed the following forms of functions f_L and f_η

$$f_L(kL) = \left(\frac{kL}{[(kL)^2 + c_L]^{1/2}} \right)^{5/3+p_0}, \quad (3.14)$$

where c_L is a positive constant and $p_0 = 2$ and

$$f_\eta(k\eta) = e^{-\beta \left\{ [(k\eta)^4 + c_\eta^4]^{1/4} - c_\eta \right\}}, \quad (3.15)$$

where $\beta = 5.2$, $c_\eta = 0.4$. If $c_\eta = 0$, Eq. (3.15) reduces to the exponential spectrum

$$f_\eta(k\eta) = e^{-\beta k\eta}, \quad (3.16)$$

where $\beta = 2.1$. An alternative model spectrum for f_η is the Pao spectrum defined as

$$f_\eta(k\eta) = e^{-\beta(k\eta)^{4/3}}, \quad (3.17)$$

where $\beta = 2.25$.

In the inertial range, the spectra follow the Kolmogorov's $-5/3$ law

$$E_{11}(k_1) = \alpha \epsilon_{PS}^{2/3} k_1^{-5/3} \quad E_{22}(k_1) = \alpha' \epsilon_{PS}^{2/3} k_1^{-5/3} \quad (3.18)$$

where $\alpha \approx 0.49$ and $\alpha' \approx 0.65$. Equations (3.18) allow to estimate the TKE dissipation rate from the inertial-range profile of the one-dimensional energy spectra.

Alternatively, the profiles of the second and third order longitudinal structure functions can be used to calculate ϵ . The n -th order structure function reads $D_n = \langle (u'_l(x+r, t) - u'_l(x, t))^n \rangle$. Here u'_l is the longitudinal component of velocity fluctuation vector. In the inertial subrange, the second and third-order structure functions are related to the dissipation rate by the formulas (e.g. [104])

$$D_2(r) = C_2 \epsilon_{D_2}^{2/3} r^{2/3}, \quad D_3(r) = -\frac{4}{5} \epsilon_{D_3} r, \quad (3.19)$$

where ϵ_{D_2} and ϵ_{D_3} should approximate ϵ .

3.3 Methods based on number of crossings

Waclawczyk et al (2017) [144] proposed two alternative methods to estimate ϵ from the number of crossings based on a restricted range of k -values available from the airborne measurements. The motivation was to possibly increase robustness of ϵ retrieval using different statistics. Their first, an indirect method, was based on the successive filtering of the signal with cut off wave-numbers k_i , where each k_i is in the inertial range. Assuming the applied filter is rectangular in the wavenumber space, then from Eqs. (3.12) and (3.18) ϵ_{NC} can be estimated from

$$\langle u_1'^2 \rangle N_1^2 - \langle u_i'^2 \rangle N_i^2 = \frac{1}{\pi^2} \int_0^{k_1} k^2 E_{11} dk - \frac{1}{\pi^2} \int_0^{k_i} k^2 E_{11} dk = 3\alpha \epsilon_{NC}^{2/3} \left(k_1^{4/3} - k_i^{4/3} \right), \quad (3.20)$$

where $\langle u_i'^2 \rangle$ is the variance and N_i is the number of crossings per unit length of a signal filtered with a cut off wave-number k_i , which is in the inertial range. Filtering the signal with a series of cut-off wave-numbers k_i , ϵ_{NC} can be estimated from Eq. (3.20) using a linear least squares fitting method, and used as a proxy for ϵ . The scaling of N_i with k_i was also investigated by Mazellier and Vassilicos (2008) [84] to estimate the dissipation rate constant C_ϵ in the Taylor's formula $\epsilon = C_\epsilon \langle u'^2 \rangle^{3/2} / \mathcal{L}$ where $\mathcal{L}$ is the longitudinal integral length scale of turbulence.

The second, iterative method was based on recovering the missing part of the spectrum in the inertial and dissipative range by introducing a correcting factor to the number of crossings per unit length N_l . As such, this method could be treated as a smooth blending between indirect and direct methods because it recovers the former as the filter cutoff moves into the inertial range and the latter as the filter cutoff moves into the dissipative range. The number of crossings per unit length N_{cut} is calculated from the low-pass filtered signal where the fine-scale fluctuations have the highest wave number k_{cut} . Assuming again that the filter is rectangular in the wavenumber space, Eq. (3.12) written for the filtered signal is

$$\pi^2 \langle u_{cut}'^2 \rangle N_{cut}^2 = \int_0^{k_{cut}} k_1^2 E_{11} dk_1, \quad (3.21)$$

where $\langle u_{cut}'^2 \rangle$ is the variance of the signal. The ratio of Eq. (3.12) and (3.21) leads to the formula

$$\langle u'^2 \rangle N_l^2 = \langle u_{cut}'^2 \rangle N_{cut}^2 \frac{\int_0^\infty k_1^2 E_{11} dk_1}{\int_0^{k_{cut}} k_1^2 E_{11} dk_1} = \langle u_{cut}'^2 \rangle N_{cut}^2 \underbrace{\left(1 + \frac{\int_{k_{cut}}^\infty k_1^2 E_{11} dk_1}{\int_0^{k_{cut}} k_1^2 E_{11} dk_1} \right)}_{\mathcal{C}_{\mathcal{F}}}, \quad (3.22)$$

where $\mathcal{C}_{\mathcal{F}}$ is the correcting factor. Assuming the energy spectrum $E(k)$ can be described by Eq. (3.13) with $f_L = 1$ and using relation (3.23) between $E(k)$ and $E_{11}(k_1)$, they obtained

$$E_{11}(k_1) = C\epsilon^{2/3} \int_{k_1}^{\infty} k^{-8/3} f_{\eta}(\beta k \eta) \left(1 - \frac{k_1^2}{k^2}\right) dk, \quad (3.23)$$

where $\beta = 2.1$, $C = 1.5$ and $\eta = (\nu^3/\epsilon)^{1/4}$ is the Kolmogorov length. Introducing (3.23) into (3.22) and changing the variables to $\xi = \beta k \eta$ and $\xi_1 = \beta k_1 \eta$, the correcting factor is obtained as

$$\mathcal{C}_{\mathcal{F}} = 1 + \frac{\int_{k_{cut}\beta\eta}^{\infty} \xi_1^2 \int_{k_1}^{\infty} \xi^{-8/3} f_{\eta}(\xi) \left(1 - \frac{\xi_1^2}{\xi^2}\right) d\xi d\xi_1}{\int_0^{k_{cut}\beta\eta} \xi_1^2 \int_{\xi_1}^{\infty} \xi^{-8/3} f_{\eta}(\xi) \left(1 - \frac{\xi_1^2}{\xi^2}\right) d\xi d\xi_1}. \quad (3.24)$$

With this, the value of dissipation rate can be estimated from Eqs. (3.10) and (3.22)

$$\epsilon_{NCR} = 15\pi^2 \nu \langle u_{cut}'^2 \rangle N_{cut}^2 \mathcal{C}_{\mathcal{F}}. \quad (3.25)$$

In order to calculate $\mathcal{C}_{\mathcal{F}}$ from Eq. (3.24), a value of η should first be specified, hence, an iterative procedure was proposed in Ref. [144]. It starts with an initial guess of the TKE dissipation rate, ϵ^0 . With this, the corresponding value of the Kolmogorov length η_0 is calculated and introduced into Eq. (3.24) for $\mathcal{C}_{\mathcal{F}}$. The TKE dissipation rate after the first iteration, ϵ^1 is found from Eq. (3.25). The procedure can be repeated, i.e. the next approximation of $\eta^1 = (\nu^3/\epsilon^1)^{1/4}$ can be calculated and substituted into Eq. (3.24). After several iterations the procedure converges to the final value of ϵ_{NCR} that should approximate ϵ with an error defined by a prescribed form $\Delta\eta = |\eta^{n+1} - \eta^n| < d_{\eta}$, where d_{η} is a given error value.

In this method, the cut-off k_{cut} may be placed in the inertial or the dissipative range. In the latter case, the spectral retrieval methods may lead to certain loss of information as they are based on the inertial-range scaling only. In Ref. [144], the performance of the new methods was tested on measurement data obtained during the physics of stratocumulus top (POST) airborne research campaign [42, 78] with the cut-off placed well in the inertial range. It was shown that the performance of the new methods was comparable with estimates from standard retrieval techniques, however, different response to errors due to finite sampling and finite averaging windows was observed. Hence, the new methods can complement the standard techniques to increase robustness of ϵ retrieval.

3.4 Alternative formulation of the iterative method

The iterative method proposed in Ref. [144] depends on the ratio of the Taylor's microscale to number of crossings microscale λ_n/Λ . In fully turbulent flows, λ_n/Λ is close to unity, see Eq. (3.6). Estimates of ϵ_{NCR} from Eq. (3.25) may be deteriorated if λ_n/Λ deviate from unity. For this reason, a different formulation of this method is proposed.

Based on Eqs. (3.3, 3.4, 3.12) and relation $\Lambda = \lambda_n = \lambda_l/\sqrt{2}$, the relation

$$\frac{1}{4} \left\langle \left(\frac{\partial u'}{\partial x} \right)^2 \right\rangle = \int_0^\infty k_1^2 E_{11} dk_1. \quad (3.26)$$

is obtained. For low-pass filtered signals (and filters rectangular in the wavenumber space), Eq. (3.26) becomes

$$\frac{1}{4} \left\langle \left(\frac{\partial u'_{cut}}{\partial x} \right)^2 \right\rangle = \int_0^{k_{cut}} k_1^2 E_{11} dk_1. \quad (3.27)$$

Hence, $\langle (\partial u'_{cut}/\partial x)^2 \rangle$ is related to $\langle (\partial u'/\partial x)^2 \rangle$ by the formula

$$\left\langle \left(\frac{\partial u'}{\partial x} \right)^2 \right\rangle = \left\langle \left(\frac{\partial u'_{cut}}{\partial x} \right)^2 \right\rangle \frac{\int_0^\infty k_1^2 E_{11} dk_1}{\int_0^{k_{cut}} k_1^2 E_{11} dk_1} = \left\langle \left(\frac{\partial u'_{cut}}{\partial x} \right)^2 \right\rangle \left(1 + \frac{\int_{k_{cut}}^\infty k_1^2 E_{11} dk_1}{\int_0^{k_{cut}} k_1^2 E_{11} dk_1} \right). \quad (3.28)$$

Introducing Eq. (3.23) for E_{11} into Eq. (3.28), the same correcting factor as in Eq. (3.24) is obtained. Based on Eqs. (3.4), (3.25) and (3.28), the value of dissipation rate is

$$\epsilon_{\lambda R} = 15\nu \left\langle \left(\frac{\partial u'}{\partial x} \right)^2 \right\rangle = 15\nu \left\langle \left(\frac{\partial u'_{cut}}{\partial x} \right)^2 \right\rangle \mathcal{C}_{\mathcal{F}}. \quad (3.29)$$

An iterative procedure, similar to the one described in section 3.3 will be used to calculate $\epsilon_{\lambda R}$. With a first guess of ϵ^0 , the correcting factor will be calculated from Eq. (3.24) and introduced into Eq. (3.29) to calculate new value of $\epsilon_{\lambda R}$. The procedure can be continued until the condition $\Delta\eta = |\eta^{n+1} - \eta^n| < d_\eta$ is satisfied.

In chapter 5, I will investigate and compare the performance of both approaches from Ref. [144] and the new one, Eq. (3.29) with different model assumptions for f_η as written in Eqs. (3.15) to (3.17) with DNS. As the DNS data contain complete information about turbulence, it will be possible to assess how the ϵ estimates change with changing cut-off wavenumber.

Chapter 4

Direct numerical simulation of atmospheric turbulence

In the study of atmospheric turbulence, the ultimate objective is to develop a workable quantitative theory or model that can be used to calculate quantities of interest and explain diverse phenomena seen in nature. It is important to reiterate some of the properties of turbulence that made it difficult to develop a model. The velocity field $\vec{u}(\vec{x}, t)$ is three-dimensional and time-dependent. There is a large range of timescales and lengthscales. The smallest Kolmogorov timescale decreases as $Re^{-1/2}$ while its lengthscale decrease as $Re^{-3/4}$. Also, difficulties arise from the convective and the pressure-gradient term in the Navier-Stokes equations.

In this chapter, my aim is to explain why the DNS data is important in the analysis of small scales in atmospheric turbulence. The two DNS datasets of atmospheric turbulence used in this thesis are summarized.

4.1 Why the use of DNS dataset is important?

Most processes observed in the atmosphere are driven by turbulence. For example, entrainment in the stratocumulus boundary layer is driven by the interaction between turbulence, evaporation, radiation and microphysics [87]. These processes are controlled not only by large turbulent eddies but also by small scale motion (characterized by turbulence kinetic energy dissipation rate ϵ). LES allows for a faster and more complete study of the parameter space, but there might be deviations between LES results and experimental data due to the absence of the small (unresolved) scales in LES. DNS resolves small-scale motions needed to investigate those processes. It also removes variability introduced by numerical artifacts and sub-grid-scale models, which complicate the interpretation of LES results. In DNS, Reynolds number is the only

parameter that does not correspond with atmospheric conditions [87, 119]. Moreover, the numerical uncertainty can be quantified easily through grid convergence studies. As a result, DNS, with a good spatio-temporal resolution, have become indispensable for studying the properties of the small-scale turbulent motion [2, 8].

4.2 Flow cases

4.2.1 Stratocumulus cloud-top simulation for DYCOMS-II RF01 case

The stratocumulus clouds have been a major focus of research in the atmospheric turbulence community because of its huge impact on the Earth’s radiative balance. This type of cloud, as compared to others (such cumulus, stratus, cirrus, cumulonimbus clouds etc.), covers about one-quarter of the Earth’s surface on average annually and play an important role in climate cooling due to its relatively high albedo [62, 78, 82]. This cloud forms at approximately 1.5 km (also referred to as low-level clouds) with a thickness of several hundred of metres. They are mostly formed over the ocean and rarely produce precipitation. The global abundance of stratocumulus clouds make it essential to accurately model and forecast their behaviour [9]. Stratocumulus-top boundary layer is caused by a strong inversion layer, which is spatially homogeneous in the horizontal directions and well mixed (during the day and night). Its turbulent structure is driven by both cloud-top radiative cooling and positive buoyancy flux from the surface [122, 134]. The structure of stratocumulus cloud-topped boundary layer is more complicated than its cloud-free counterpart because of the strong interaction between turbulent motions, radiative fluxes and cloud microphysics [86, 122].

To study the stratocumulus-top boundary layer, a cloud-top mixing layer simulation (cf. figure 4.1 and 4.2) is considered as a test case. This system mimics the cloud-top region of stratocumulus clouds and proves convenient to study some aspects associated with submeter scales, like evaporative cooling, since simulations of the complete boundary layer cannot reach these small grid spacings. The cloud-top mixing layer consists of two infinite horizontal layers of moist air: the upper region, which is warm and unsaturated, and the lower region, which is cool and saturated (condensate-laden). Longwave radiative cooling of the upper region of the cloud leads to convective instability, and this instability is a major source of cloud turbulence. Radiative cooling is characterized by the net upward radiative flux F_0 and the radiative extinction length L_0 , over which that cooling concentrates. The first research flight of the DYCOMS II field campaign and its measurement-based estimates $L_0 = 15$ m and

$F_0 = 70 \text{ W m}^{-2}$ are used as reference in this simulation [134]. These radiative properties imply a reference buoyancy flux $B_0 = F_0 g / (\rho c_p T_0) = 0.002 \text{ m}^2 \text{ s}^{-3}$, where g is the gravitational acceleration, and a reference velocity scale $U_0 = (B_0 L_0)^{1/3} = 0.3 \text{ m s}^{-1}$. The Reynolds number in the simulation is $U_0 L_0 / \nu = 800$, which is about 300 times smaller than that in the atmosphere. Consequently, there is a need to assess the effect of the low Reynolds number in the results. In addition to the radiative forcing, the evaporative cooling induced by the mixing of cloudy and environmental air, and the wind-shear effects induced by a velocity variation along the cloud-top region of 3 m s^{-1} are retained [36]. The governing equations used for this simulation are written in equations (2.10) to (2.14).

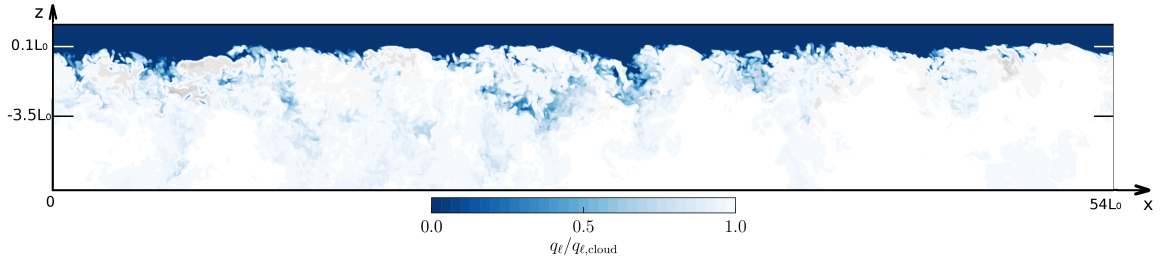


Figure 4.1: Vertical cross section of the liquid water specific humidity in the cloud-top mixing layer. Gray colors indicate regions with q_l higher than inside the cloud due to the radiative cooling. The horizontal bars at the sides of the figure indicate the position of the minimum buoyancy flux (horizontal plane $z = 0.1L_0$, where L_0 is the radiative extinction length) and the maximum buoyancy flux (horizontal plane $z = -3.5L_0$) [119].

The horizontal size of the computational domain is $54 L_0$. The domain is discretized with $5120 \times 5120 \times 2048$ points in the streamwise, spanwise and vertical directions, which assures fine resolution of the flow down to the smallest dissipative eddies with a characteristic size $\eta_0 = (\nu^3/B_0)^{1/3} \simeq 10 \text{ cm}$. The system is statistically homogeneous inside the horizontal planes, and the data inside these planes are used to construct the different statistics, which depend on the vertical coordinate z and the time t . Further details of the simulations can be found in Ref. [119]. I investigate the three velocity components in four horizontal planes at heights $z \in \{-5.2L_0, -3.5L_0, -1.7L_0, 0.1L_0\}$, where $z = 0.1L_0$ corresponds to the height of minimum buoyancy flux and $z = -3.5L_0$ corresponds to the height of maximum buoyancy flux.

Figure 4.3 includes vertical profiles of the mean velocity, $\langle u \rangle$ in the streamwise (x) direction, the root-mean-square (r.m.s.) of the three velocity components u_{rms} , v_{rms} and w_{rms} in the streamwise, spanwise and vertical directions, respectively and

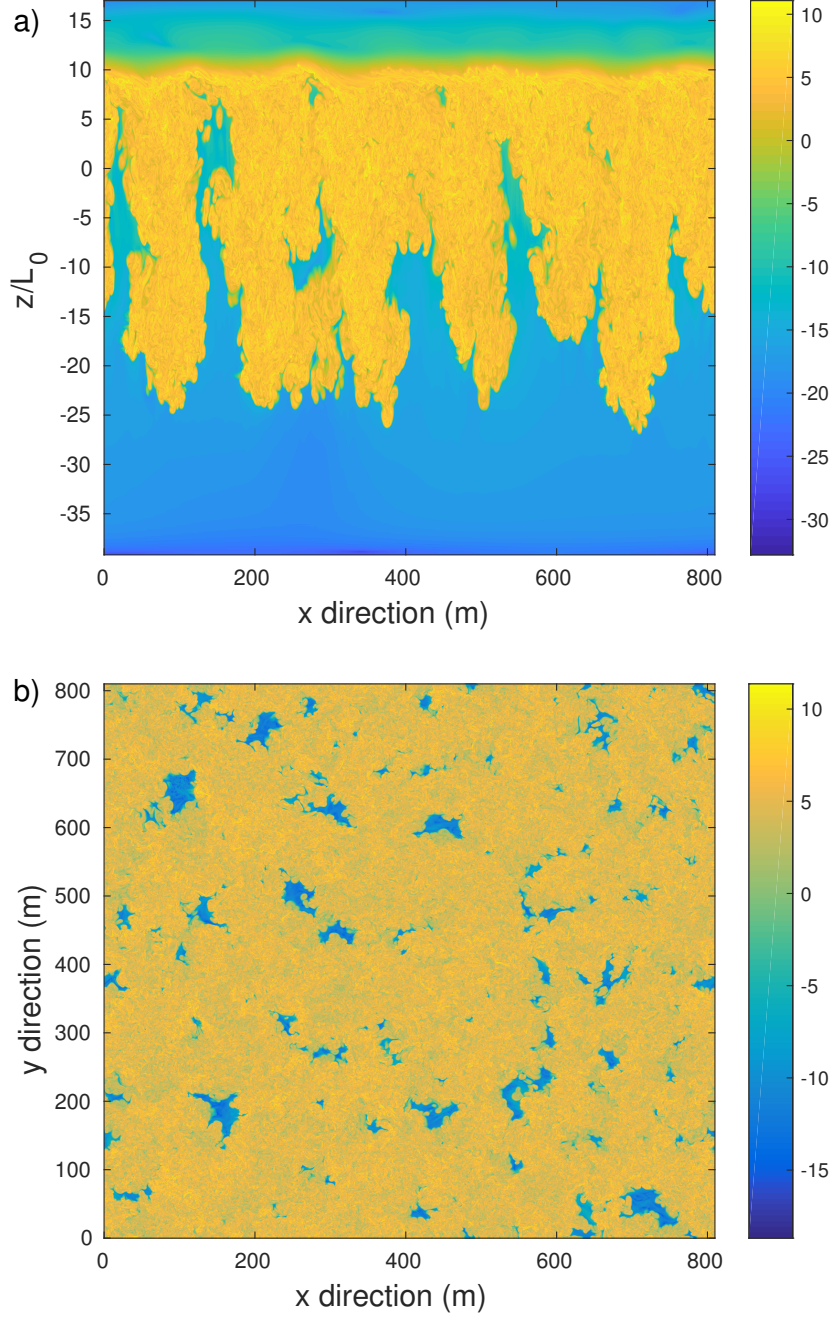


Figure 4.2: Logarithm of enstrophy ($\Omega = 1/2|\boldsymbol{\omega}|^2$ where $\boldsymbol{\omega}$ is the vorticity field). (a) Vertical cross section at $y = 405\text{m}$. (b) Horizontal cross section at $z = -3.5L_0$ [119].

the budget of the turbulence kinetic energy. The angle brackets indicate horizontal average. The viscous dissipation rate of the turbulence kinetic energy is defined by equation 3.1, the buoyancy flux is $B = \langle b'w' \rangle$, and the shear production term is $P = -\langle u'w' \rangle \partial_z \langle u \rangle$. It is worth to comment that profiles of r.m.s. velocity component

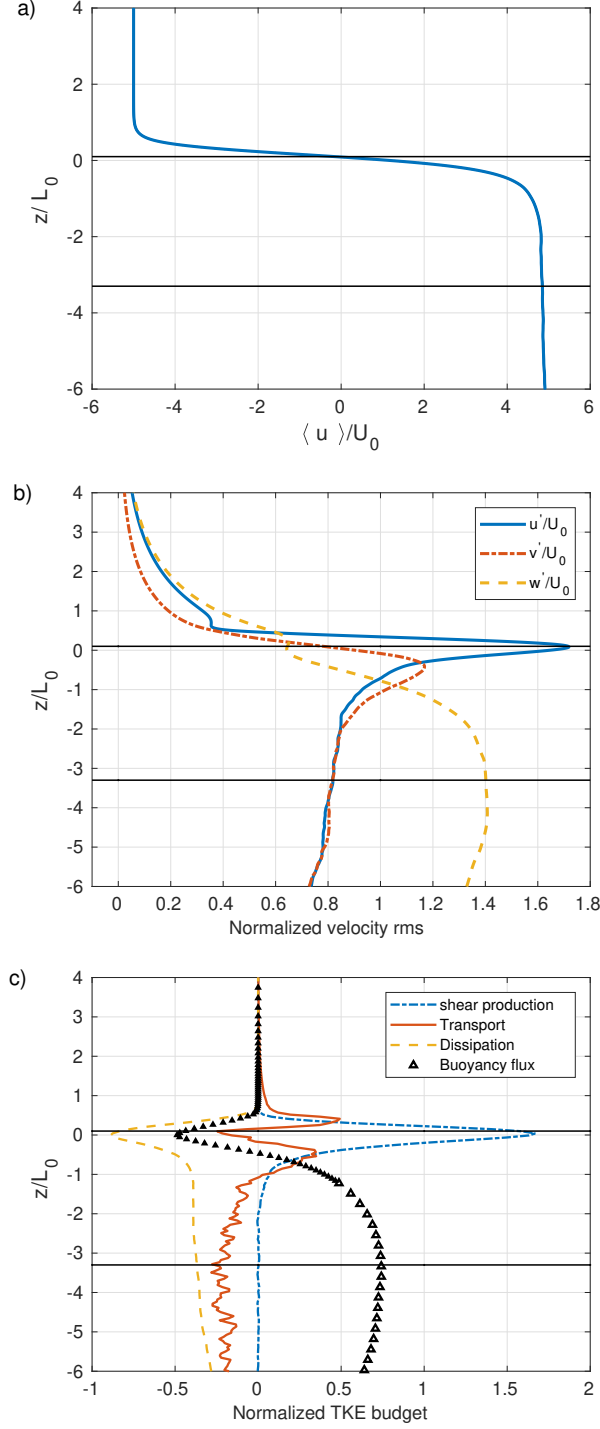


Figure 4.3: Some statistics of velocity field in the cloud-top mixing layer. The upper horizontal line indicates the height of minimum buoyancy flux (horizontal plane $z = 0.1L_0$) while the lower horizontal black line indicates the height of maximum buoyancy flux (horizontal plane $z = -3.5L_0$) [119].

fluctuations in figure 4.3 indicating anisotropy of turbulence are in agreement with the measurement data reported in Ref. [55]. Moreover, profiles of budget terms of turbulence kinetic energy are in agreement with observations reported in Ref. [27] and results of high-resolution large eddy simulations (LES) [49, 66].

4.2.2 Free convective boundary layer

Free convection occurs in an unstable planetary boundary layer (see figure 4.4) when there is a relative turbulent motion between the surface and the atmosphere, caused by strong surface heating, weak mean horizontal flow and buoyancy force. Understanding the evolution and properties of free convection are important for the accurate parameterization in global climate models [89]. Numerous authors have studied the free convective boundary layer (CBL) in field campaigns (see Ref. [4, 158]) and laboratory studies (see Ref. [3, 85]) and LES (see Ref. [93]).

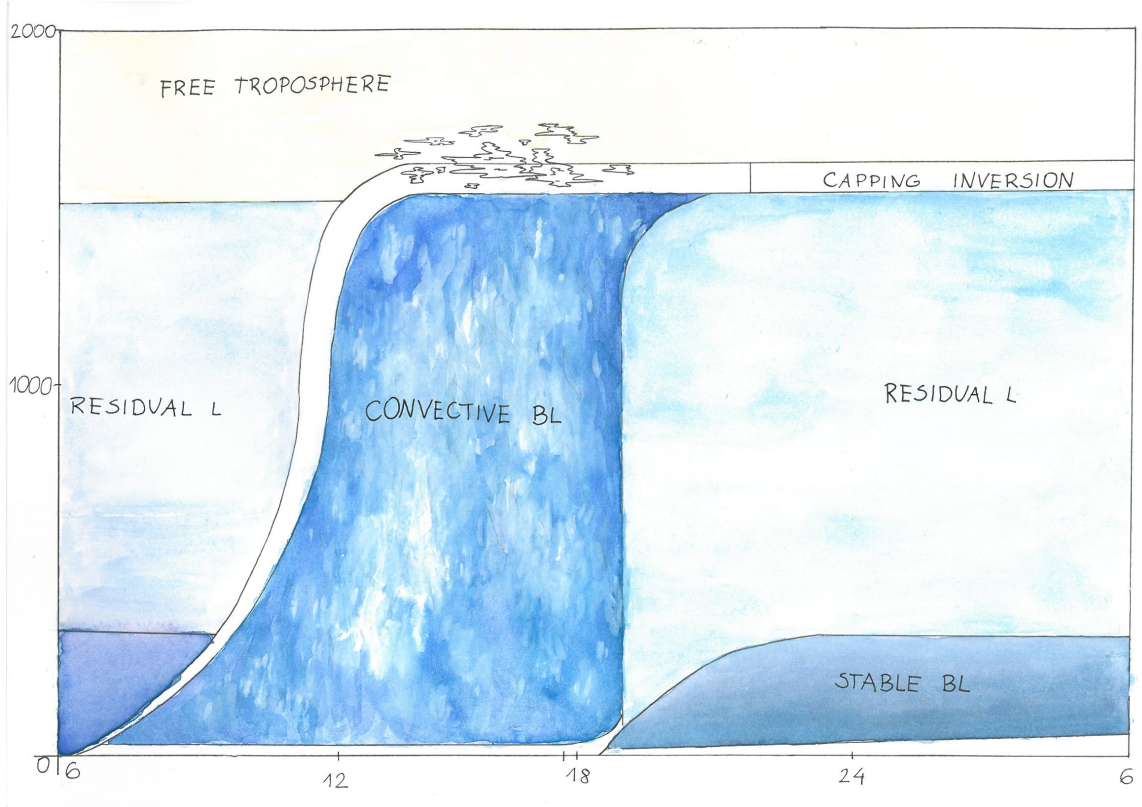


Figure 4.4: Diurnal cycle of the planetary boundary layer, showing the free convective boundary layer. Courtesy to Z. Waławczyk and adapted from Ref. [30].

The simulation considers a dry, shear-free CBL that grows into a linearly stratified atmosphere (cf. figure 4.5). The flow is driven by a constant and homogeneous

surface buoyancy flux B_0 , and the buoyancy stratification of the free atmosphere is N^2 , where N is the buoyancy frequency. This configuration is representative of midday atmospheric conditions over land.

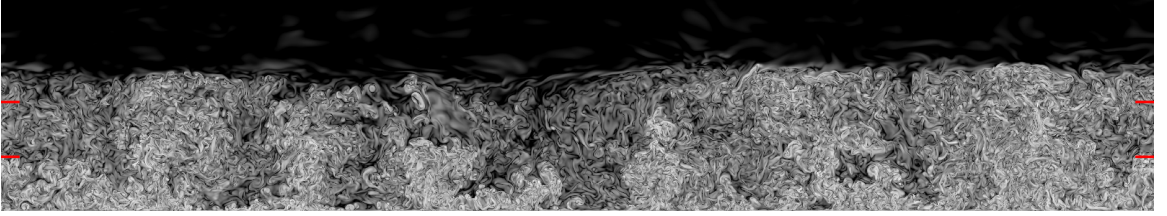


Figure 4.5: Vertical cross section of the logarithm of the enstrophy in the convective boundary layer [89]. The horizontal bars at the side of the figures indicate a height equal to the CBL depth h and equal to half of it.

After the initial conditions have been sufficiently forgotten, statistical properties can be expressed as a function of the buoyancy Reynolds number $Re_0 = B_0/(\nu N^2)$, the normalized vertical distance to the surface z/h , and the normalized time tN . Instead of time, the ratio h/L_0 is often used. The variable $h(t)$ is defined as

$$h = \left(2N^{-2} \int_0^{z_\infty} (\langle b \rangle - N^2 z) dz \right)^{1/2} \simeq (2B_0 N^{-2} t)^{1/2} \quad (4.1)$$

and provides a measure of the CBL depth. The symbol b indicates the buoyancy and the last approximation is derived from the integral analysis of the advection-diffusion evolution equation for the buoyancy. The parameter $L_0 = (B_0/N^3)^{1/2}$ is the reference Ozmidov scale and provides a measure of the thickness of transition layer at the top of the entrainment zone between the turbulent boundary layer and the free atmosphere [41]. The ratio h/L_0 increases as the CBL grows into the linearly stratified atmosphere and h/L_0 varies between 5 and 50 for typical midday conditions. Beyond $h/L_0 \simeq 10 - 15$, the CBL is in a quasi-steady regime in which CBL properties evolve on time scales much larger than the eddy turnover time of the large, energy-containing motions. The simulation was performed using the Boussinesq approximation described in equations (2.5) to (2.7).

The simulation dataset with a buoyancy Reynolds number Re_0 equal to 117 and at a state of development $h/L_0 \simeq 21.5$ is for the analysis. The number of grid points used in the simulation are $5120 \times 5120 \times 1024$, in the streamwise, spanwise and vertical directions, respectively. Further details can be found in Mellado et al. (2016) [89]. For the analysis presented here, five horizontal planes, namely, $z \in \{0.29h, 0.43h, 0.71h, 1.0h, 1.14h\}$ is used. The height $z = 1.14h$ corresponds to the height of minimum buoyancy flux.

Chapter 5

Analysis of TKE dissipation rate with different retrieval techniques

This chapter provides a study on the performance of different retrieval techniques outlined in chapter 3 in comparison with the actual value from DNS. I use the stratocumulus cloud top and free convective boundary layer simulation datasets in this analysis. Both simulation datasets were provided by *Professor Juan Pedro Mellado - Max Planck Institute for Meteorology*. All analyses were done with MATLAB® software.

5.1 TKE dissipation rate estimates from inertial-range scaling

The methods related to the local isotropy assumption and inertial-range scaling are commonly used to analyse 1D signals from airborne measurements. At the same time, turbulent flows in clouds or atmospheric boundary layers are inhomogeneous and buoyant. The purpose of this analysis is to check how predictions of these methods, when applied to DNS data, compare with the true value of ϵ_{DNS} calculated from Eq. (3.1).

5.1.1 Analysis with the stratocumulus cloud-top simulation data

First, 1D spectra of three velocity components u , v and w on horizontal cross-sections through the computational domain are investigated, see Figs. 5.2, 5.3 and 5.4, respectively. In order to calculate the compensated spectra, each E_{11} , E_{22} and E_{33} were multiplied by $\epsilon_{DNS}^{-2/3}$ at $z \in \{-5.2L_0, -3.5L_0, -1.7L_0, 0.1L_0\}$ (see figure 5.1) and by

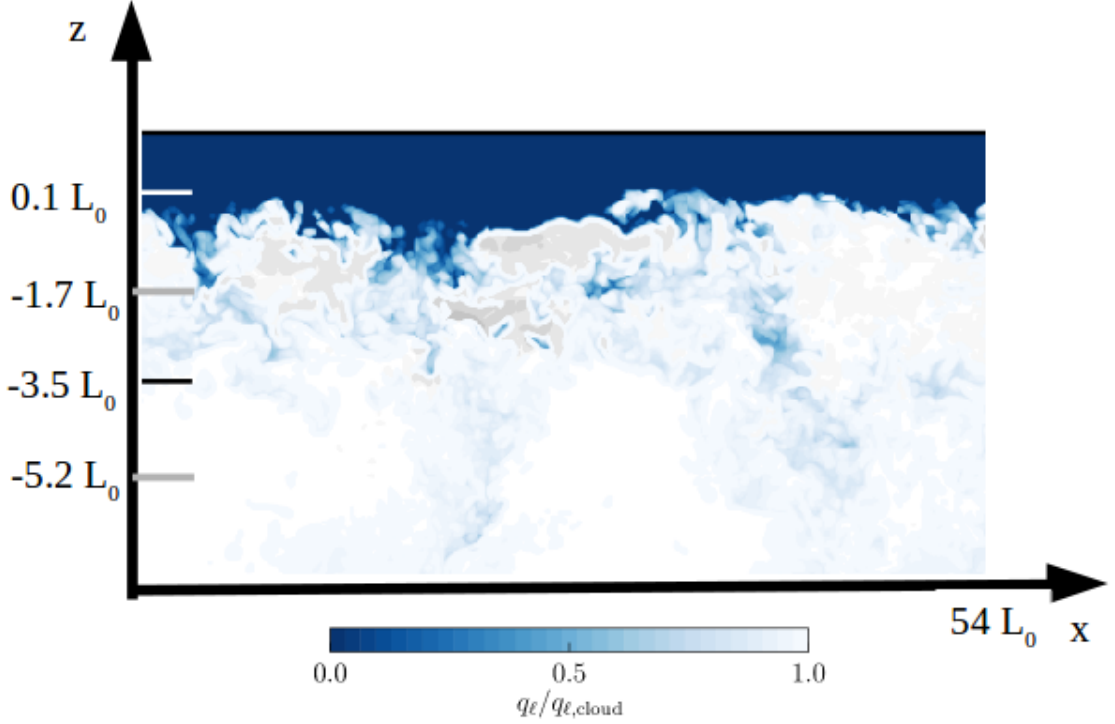


Figure 5.1: Vertical cross section of the liquid water specific humidity in the cloud-top mixing layer showing horizontal plane $z = -5.2L_0, -3.5L_0, -1.7L_0, 0.1L_0$.

$k_1^{5/3}$ or $k_2^{5/3}$. Spectra calculated in x direction were additionally averaged in the span-wise y direction. Similarly, spectra calculated in y direction were averaged in the streamwise x direction. The horizontal lines in Figs. 5.2, 5.3 and 5.4 are equal to the constant coefficients from Eq. (3.18), $\alpha = 0.5$ for the longitudinal and $\alpha' = 0.65$ for the transverse spectra. These constant coefficients were obtained from theoretical analysis and experimental data [104, 131].

Similar profiles of corresponding compensated spectra at planes $z = -5.2L_0, -3.5L_0, -1.7L_0$ are observed. The profiles calculated at plane $z = 0.1L_0$, placed in the upper part of stratocumulus cloud are clearly different. This region of the flow is affected by the presence of shear, stable stratification (see Fig. 4.1) as well as external intermittency. Moreover, differences are observed between different types of spectra. The longitudinal ones, $E_{11}(k_1)$ and $E_{22}(k_2)$ (Figs. 5.2a and 5.3b) seem to follow the Kolmogorov's K41 theory quite closely in a certain range of wavenumbers. This is in spite of the relatively low- Re number of the considered flow, where a clear separation between the dissipative and energy-containing scales may not be attained. At the same time, the transverse spectra $E_{11}(k_2)$ and $E_{22}(k_1)$ (Figs. 5.2b and 5.3a) seem to scale with $\sim k_1^{-a}$ or k_2^{-a} where a is somewhat smaller than $5/3$. Interestingly,

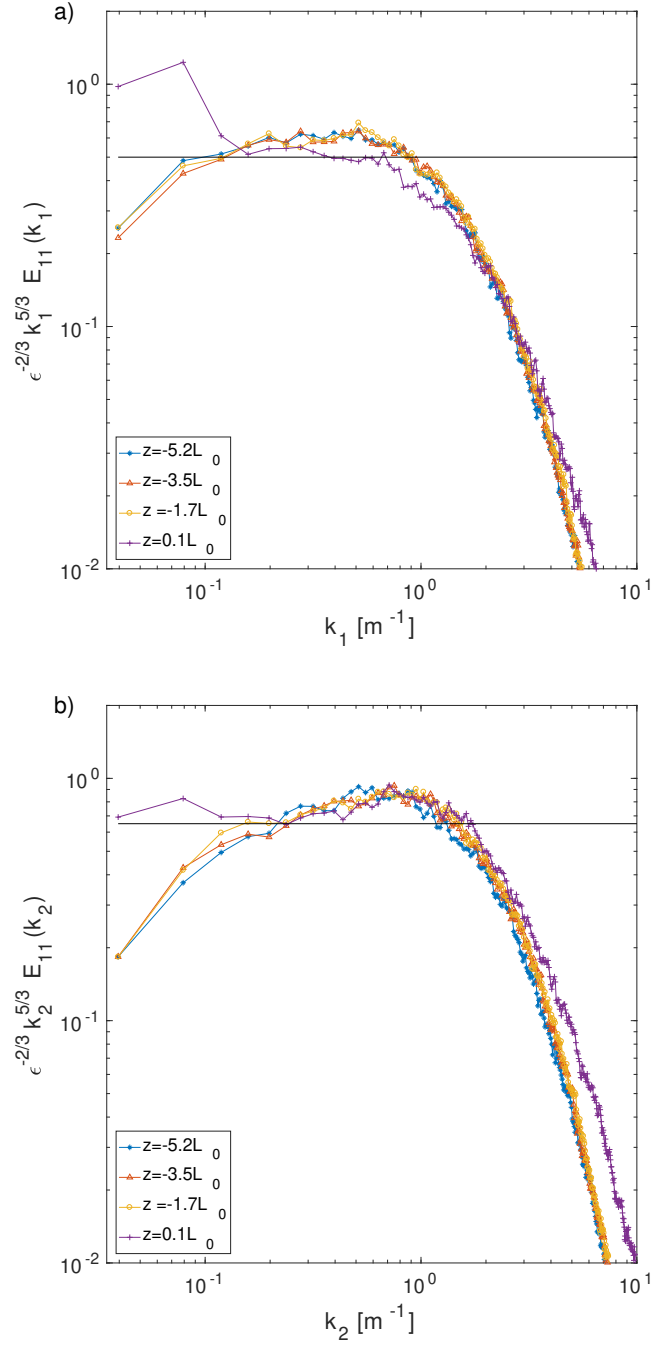


Figure 5.2: Compensated 1D velocity spectra (dimensionless) of the u velocity component at $z \in \{-5.2L_0, -3.5L_0, -1.7L_0, 0.1L_0\}$ a) longitudinal, b) transverse.

inertial range with the scaling close to $k_1^{-5/3}$ and $k_2^{-5/3}$ can be distinguished for the transverse spectra of the third velocity component in Fig. 5.4, however, the constant $\alpha' \approx 1$ is larger than the value 0.65 predicted by the Kolmogorov's theory. Spectral anisotropy of velocity component structure at $z = 0.1L_0$ layer, indicate the role of

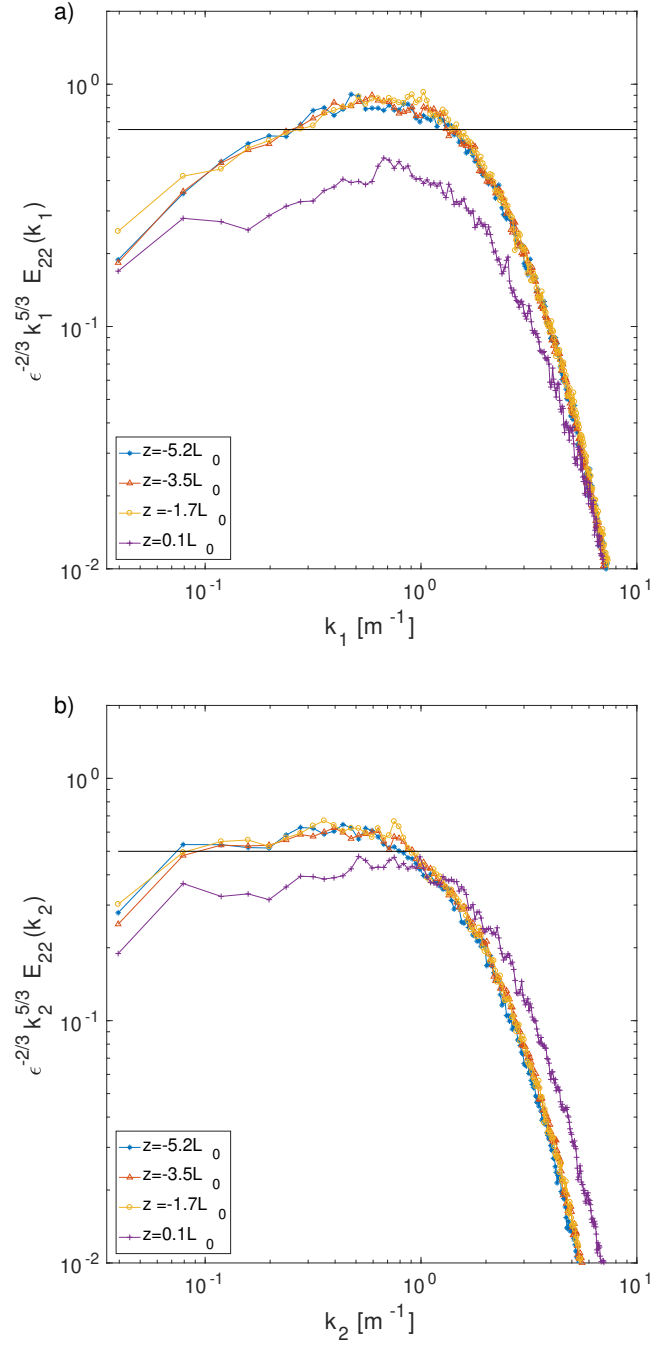


Figure 5.3: Compensated 1D velocity spectra (dimensionless) of the v velocity component at $z \in \{-5.2L_0, -3.5L_0, -1.7L_0, 0.1L_0\}$ a) transverse, b) longitudinal.

stable stratification above the cloud top and is in agreement with the experimental data and LES simulations reported in Ref. [99].

In the following, the extent to which the deviations from the K41 theory (observed in figures 5.2-5.4) affect estimations of ϵ will be studied. To estimate ϵ_{PS} from power

	k - fitting range	$\frac{\epsilon_{PS}}{B_0}$	$\frac{\epsilon_{NC}}{B_0}$	k - fitting range	$\frac{\epsilon_{PS}}{B_0}$	$\frac{\epsilon_{NC}}{B_0}$	$\frac{\epsilon_{D_2}}{B_0}$	$\frac{\epsilon_{D_3}}{B_0}$	$\frac{\epsilon_{SR}}{B_0}$	Λ/λ_n	$\frac{\epsilon_\Lambda}{B_0}$
u in x	0.17 - 0.63	0.47	0.42	0.49 - 0.85	0.41	0.31	0.31	0.23	0.26	1.17	0.37
v in y	0.25 - 0.63	0.47	0.40	0.42 - 0.84	0.43	0.33	0.32	0.21	0.26	1.17	0.37
u in y	0.29 - 0.84	0.50	0.40	0.84 - 1.67	0.38	0.26	0.30		0.24	1.24	0.37
v in x	0.33 - 0.63	0.52	0.41	0.75 - 1.38	0.43	0.29	0.28		0.22	1.24	0.37
w in x	0.25 - 0.63	0.65	0.51	0.33 - 0.59	0.63	0.48	0.57		0.27	1.22	0.40
w in y	0.17 - 0.63	0.65	0.55	0.33 - 0.59	0.64	0.52	0.58		0.28	1.20	0.40

Table 5.1: Values of dissipation rate calculated for horizontal plane $z = -3.5L_0$, ϵ_{PS} , ϵ_{NC} , ϵ_{D_2} , ϵ_{D_3} , ϵ_{SR} and ϵ_Λ , are the dissipation rates calculated from Eq. (3.2), Eq. (3.18), Eq. (3.20), Eqs. (3.19) and Eqs. (3.10,3.11), respectively. $\epsilon_{DNS} = 0.36B_0$ is the averaged instantaneous dissipation rate from DNS and Λ/λ_n is the ratio of zero crossing micro-scale to Taylor's micro-scale. The first fitting ranges seemed optimal for power spectra, the second - for structure functions.

	k - fitting range	$\frac{\epsilon_{PS}}{B_0}$	$\frac{\epsilon_{NC}}{B_0}$	k - fitting range	$\frac{\epsilon_{PS}}{B_0}$	$\frac{\epsilon_{NC}}{B_0}$	$\frac{\epsilon_{D_2}}{B_0}$	$\frac{\epsilon_{D_3}}{B_0}$	$\frac{\epsilon_{SR}}{B_0}$	Λ/λ_n	$\frac{\epsilon_\Lambda}{B_0}$
u in x	0.21 - 0.42	0.91	0.58	0.11 - 0.21	0.93	0.73	1.65	1.20	0.33	1.35	0.64
v in y	0.42 - 0.84	0.72	0.63	0.23 - 0.46	0.64	0.37	0.89	0.45	0.45	1.31	0.79
u in y	0.42 - 0.84	1.16	0.97	0.71 - 2.09	0.39	0.16	0.25		0.51	1.28	0.84
v in x	0.46 - 0.55	0.40	0.33	0.71 - 2.09	0.94	0.87	0.77		0.17	1.46	0.38
w in x	0.42 - 0.84	0.37	0.22	0.13 - 0.67	0.23	0.20	0.18		0.16	1.51	0.36
w in y	0.84 - 1.64	0.57	0.29	0.80 - 1.33	0.51	0.29	0.27		0.30	1.56	0.73

Table 5.2: Values of dissipation rate calculated for horizontal plane $z = 0.1L_0$, ϵ_{PS} , ϵ_{NC} , ϵ_{D_2} and ϵ_{D_3} , ϵ_{SR} , ϵ_Λ are the dissipation rates calculated from Eq. (3.2), Eq. (3.18), Eq. (3.20), Eqs. (3.19) and Eqs. (3.10,3.11), respectively. $\epsilon_{DNS} = 0.89B_0$ is the averaged instantaneous dissipation rate from DNS and Λ/λ_n is the ratio of zero crossing micro-scale to Taylor's micro-scale. The first fitting ranges seemed optimal for power spectra, the second - for structure functions.

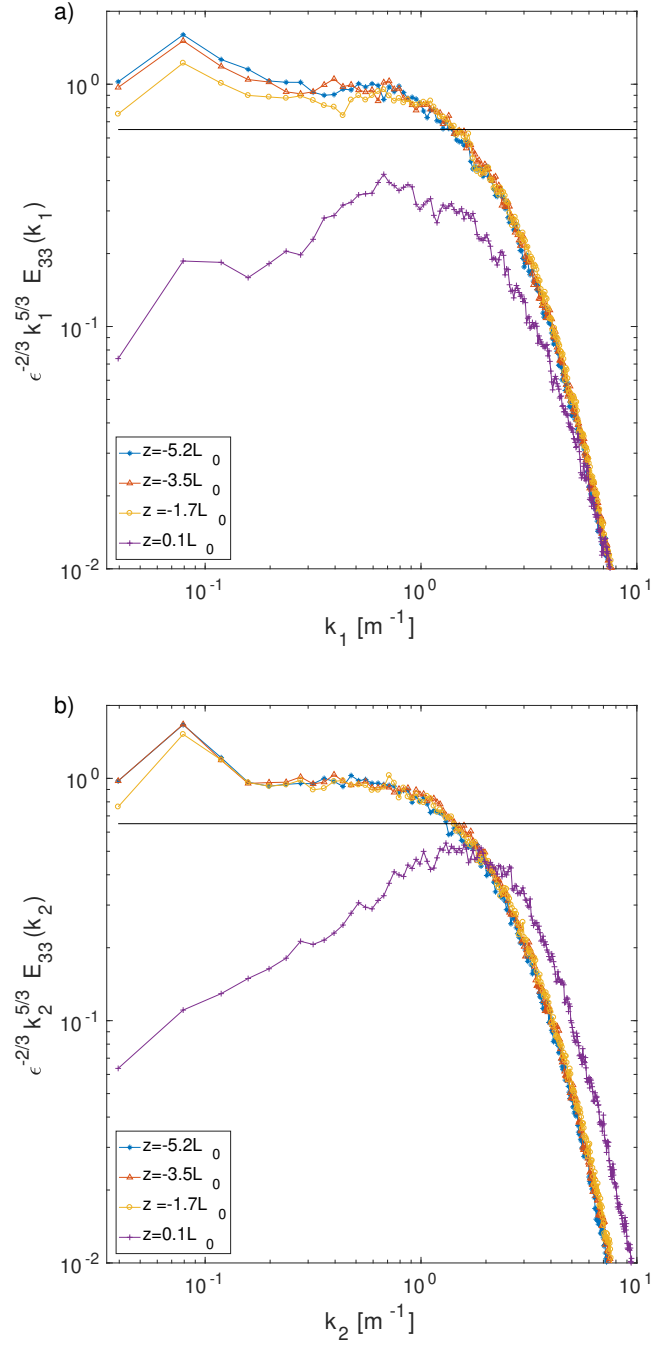


Figure 5.4: Compensated 1D velocity spectra (dimensionless) of the w velocity component at $z \in \{-5.2L_0, -3.5L_0, -1.7L_0, 0.1L_0\}$ a) transverse in x direction, b) transverse in y direction.

spectra (Eqs. 3.18), we fit a line with $-5/3$ slope on a logarithmic plot. The log of the intercept is equivalent to $\alpha\epsilon_{PS}^{2/3}$ or $\alpha'\epsilon_{PS}^{2/3}$. Figure 5.5 provides the scaling of $N_i^2\langle u_i'^2 \rangle$ with filter cut-off k_i and $k_1 = 0.4 \text{ m}^{-1}$, see Eq. (3.20). The sixth order Butterworth

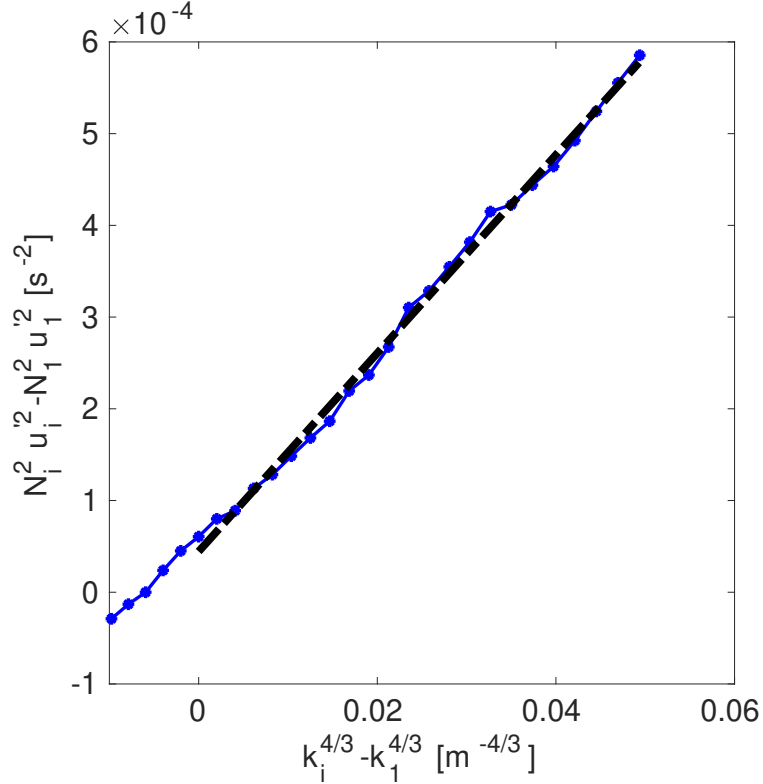


Figure 5.5: Corresponding scaling of $u_1'^2 N_1^2$ with filter cut-off k_i . The fits are given by black lines.

filter was used to calculate successive u'_{cut} . For a given $k_{cut} = k_i$, a corresponding number of crossings N_i was calculated for a filtered signal u'_{cut} . The linear fit slope is equivalent to $3\alpha\epsilon_{NC}^{2/3}$ in which the dissipation rate ϵ_{NC} was calculated.

Next, ϵ from the second and third order structure functions is estimated, as written in Eq. (3.19) [104]. Inertial range values were obtained by fitting linearly a slope of $2/3$ to the second order structure function as shown in figure 5.6. The intercept of this fit is used to get the value of ϵ_{D_2} from the second-order structure function (ϵ_{D_2}). Analogous procedure is performed to calculate ϵ_{D_3} .

In case of homogeneous, isotropic turbulence, all estimates of ϵ from power spectrum, second- and third-order structure functions should, theoretically, be equal. It would hence seem appropriate to use the same fitting ranges for ϵ_{PS} , ϵ_{D_2} and ϵ_{D_3} , just appropriately converted from k -space to r -space (i.e. with $k = 2\pi/r$). In practice, the choice of fitting ranges was difficult due to the short inertial ranges (cf. figure 5.5) - an attribute of low Reynolds number flows. This makes the spectral retrieval estimates difficult and much dependent on the chosen fitting range. As pointed out in Ref. [51] and confirmed by other authors (e.g see [29]), the effect of finite power law

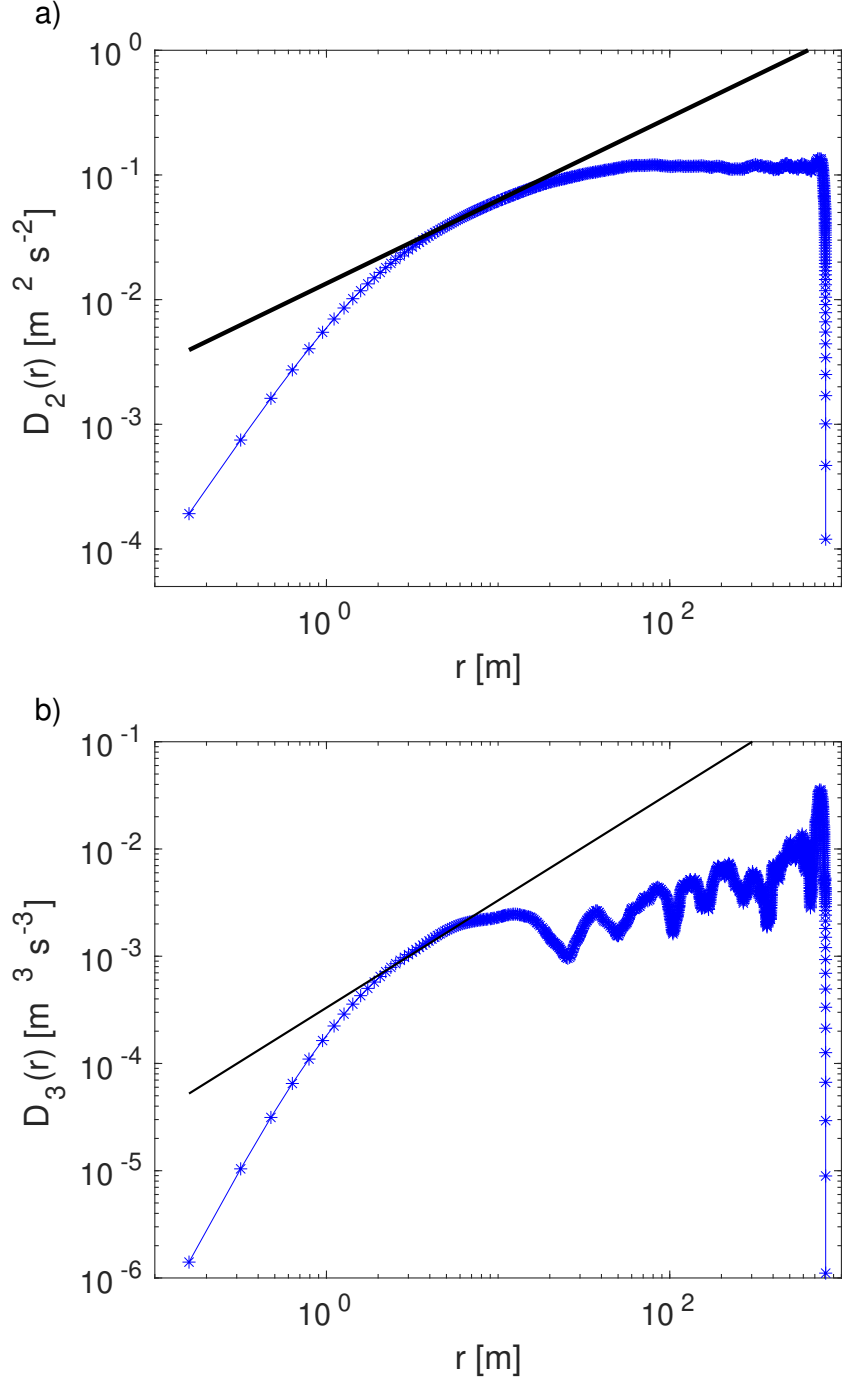


Figure 5.6: Second- and third- order structure function of u in x at horizontal plane $z = -3.5L_0$ showing the linear fit of a) $\sim r^{2/3}$, b) $\sim r^1$.

range in the spectral space results in a much shorter power law range in the physical space. Also, in our case, the fitting ranges optimal for D_2 , were different from those for power spectra. To show difference in the estimates, I compare, in detail, results of different methods and different fitting ranges for planes $z = -3.5L_0$ and $z = 0.1L_0$,

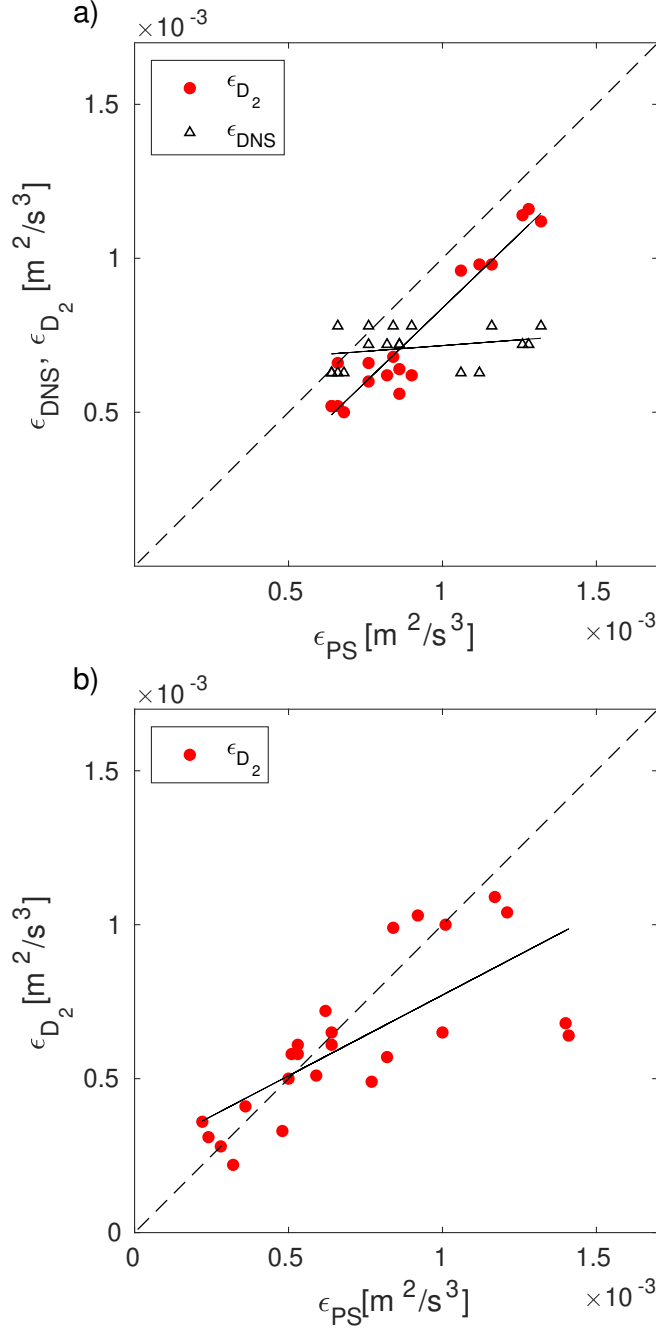


Figure 5.7: TKE dissipation rates in CTL ϵ_{PS} vs. ϵ_{D_2} (red circles) and ϵ_{PS} vs. ϵ_{DNS} in the well-mixed cloud top layer a) stratocumulus cloud top simulation, b) POST measurements [55].

because they are regions of maximum and minimum buoyancy flux, respectively. The plane $z = -3.5L_0$ is placed in the turbulent region inside the cloud. The true value of ϵ at this plane equals $\epsilon_{DNS} = 0.36B_0$.

Next, results of indirect methods based on the inertial-range scaling are presented

in Table 5.1. The first fitting range seemed to be optimal for the investigated spectra. First, TKE dissipation rate estimates ϵ_{PS} based on Eq. (3.18) and estimates from number of crossing scaling in the inertial range ϵ_{NC} , Eq. (3.20) are considered.

The second fitting range presented in Table 5.1 seemed optimal for the second-order structure functions D_2 . ϵ estimates based on power spectrum ϵ_{PS} , number of crossings ϵ_{NC} , second and third order structure functions ϵ_{D_2} and ϵ_{D_3} from Eqs. (3.19), all calculated for the second fitting range were presented. Certain discrepancy of results is observed, also between ϵ_{PS} and ϵ_{D_2} which are standard methods of estimating TKE dissipation rate. Moreover, ϵ_{PS} are over-predicted and ϵ_{D_2} , ϵ_{D_3} , ϵ_{NC} are under-predicted when compared to $\epsilon_{DNS} = 0.36B_0$. Table 5.2 shows the corresponding fits for the horizontal profile $z = 0.1L_0$. The plane $z = 0.1L_0$ is placed in the upper part of the stratocumulus cloud, in the region affected by the stable stratification, high shear and external intermittency. Hence, the discrepancy between ϵ_{DNS} and estimates from velocity signals is larger. Results differ also between the horizontal velocity components (u in x , u in y , v in x and v in y). This concerns even ϵ_λ estimates which makes the local isotropy assumption questionable. Moreover, the calculated ratios Λ/λ_n are very large. Such large values were also reported in Ref. [57] in the upper part of the boundary layer, affected by external intermittency. This leads to the idea that Λ/λ_n is an indicator of external intermittency, which will be described in more detail in Section 5.2.3.

The TKE dissipation rate estimates from 1D signals: ϵ_{PS} , ϵ_{D_2} and ϵ_{DNS} at planes $z = -1.7L_0, -3.5L_0, -5.2L_0$ are compared in Fig. 5.7a. The fitting ranges were chosen to match the inertial range of structure functions. It is seen that ϵ_{D_2} are in most cases smaller than ϵ_{PS} . An underprediction of ϵ_{D_2} vs. ϵ_{PS} was also observed in the cloud-top POST measurements [55] of stratocumulus clouds in the well-mixed cloud-top layer (therein called CTL). Results from POST for this part of the cloud are presented in Fig. 5.7b. It can be concluded that similarities exists between results presented in Figs. 5.7a and 5.7b. At the same time, having exact DNS data at hand, it is seen that the true ϵ_{DNS} dissipation rate is yet different, see Fig. 5.7a.

As it is seen in Tables 5.1 and 5.2, the estimates of ϵ from the vertical velocity component w differ from those based on horizontal components. This seems to withstand the local isotropy assumption at inertial-range scales. Moreover, ϵ estimates based on w are much overpredicted in comparison to ϵ_{DNS} at plane $z = -3.5L_0$ which is placed inside the CTL, where buoyancy is a source of turbulence generation (see Table 5.1) and underpredicted at plane $z = 0.1L_0$ (see Table 5.2) where the negative buoyancy damps the vertical velocity fluctuations. In the analysis of POST data, this layer of

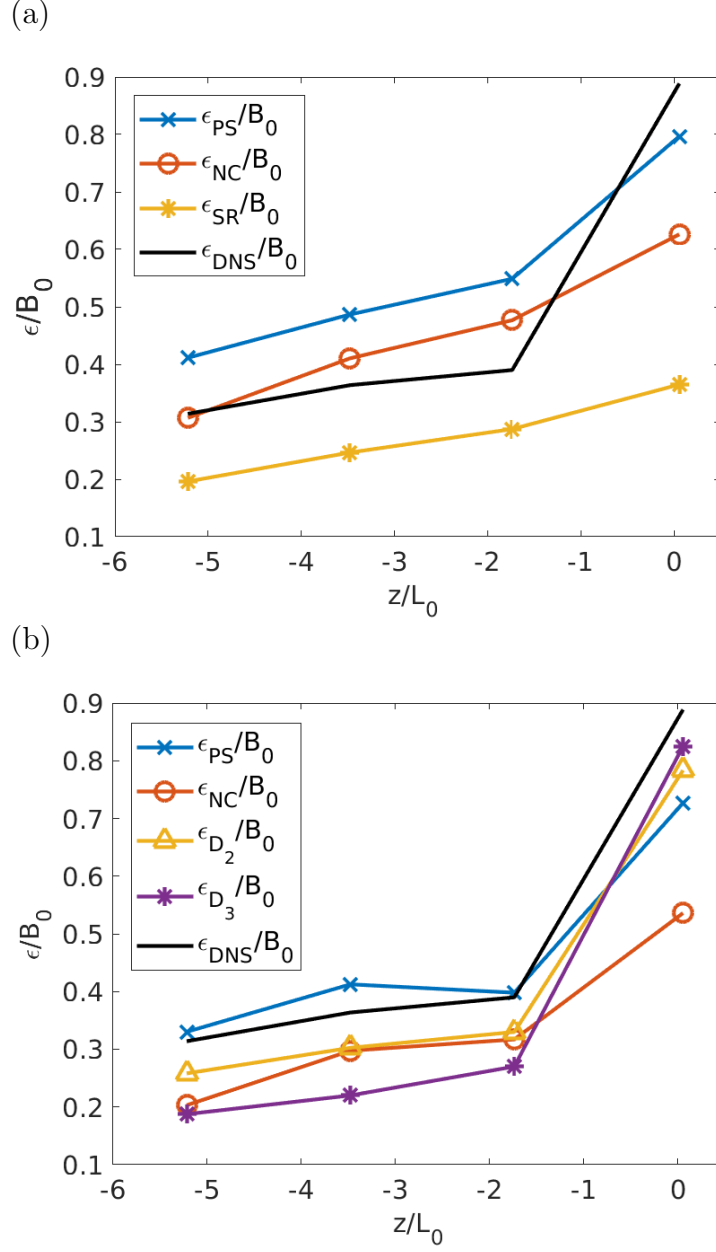


Figure 5.8: Average TKE dissipation rates for stratocumulus cloud top simulation calculated from Eq. (3.18), Eq. (3.20) and Eqs. (3.10, 3.11) (a) Fitting ranges were estimated based on E_{11} and E_{22} functions, b) Fitting ranges were estimated based on D_2 function.

the cloud was referred to as moist and sheared cloud top mixing sublayer (CTMSL) [55] and, likewise, ϵ estimates based on w were underpredicted in this region as com-

pared to estimates from u (see Fig. 7 therein). On the contrary, measurements in cumulus clouds reported in Ref. [126] seem to confirm the local isotropy assumption. Therein, the authors argue that at least to decimeter scales, turbulence in cumulus clouds can be well described with the same methods as used for cloud-free conditions.

In the remaining part of this analysis, ϵ was estimated using the 4 signals with horizontal velocity components, which allows to obtain results much closer to ϵ_{DNS} . I first use both inertial ranges and compare their ϵ estimates (averaged over 4 signals u in x , u in y , v in x and v in y) in figures 5.8a and 5.8b.

Comparing figures 5.8a and 5.8b, the structure function's fitting ranges give better estimates. The number of crossing method Eq. (3.20) agrees closely with second-order structure function for $z = -1.7L_0, -3.5L_0, -5.2L_0$. The results of ϵ_{D_3} from third-order structure function are underestimates (also reported in Ref. [29]), which is contrary to the idea that these estimates is preferable due to its analytically derived constant (4/5). The maximum value of TKE dissipation rate was found at the cloud top mixing sublayer, which agrees with the experiment from Ref. [55]. However, what can be seen, especially from 5.8a is that ϵ values estimated from the inertial-range arguments in this non-isotropic, shear-influenced part of the cloud can be much underpredicted in comparison to the true TKE dissipation rate value. The buoyancy flux is positive at heights $z = -5.2L_0, -3.5L_0, -1.7L_0$ of stratocumulus-top simulations. At $z = 0.1L_0$, the negative buoyancy flux damps vertical velocity component fluctuations.

5.1.2 Analysis with the free convective boundary layer

The same analysis of section 5.1.1 was performed to the DNS of free CBL [89]. Although, a different flow case than in Section 5.1.1 is considered, one-dimensional spectra shown in Figs. 5.10-5.12 are similar to the corresponding plots 5.2-5.4. The inertial range scaling $\sim k_1^{-5/3}$ or $\sim k_2^{-5/3}$ can be best recognised for the longitudinal spectra in Figs. 5.10a and 5.11b and for the transverse spectra of the vertical velocity component in Fig. 5.12. In this latter case, however, the proportionality constant again exceeds the isotropic value $\alpha' = 0.65$, similarly as in the corresponding Fig. 5.4 for the stratocumulus cloud. Profiles calculated at the height of minimum buoyancy flux, corresponding to $z = 1.14h$ (see figure 5.9) compare better with the remaining spectra than it was the case for stratocumulus-top simulations (therein, layer $z = 0.1L_0$). Based on Figs. 5.2-5.4 and 5.10-5.12, the observed deviations from the Kolmogorov's scaling are caused by the anisotropy of the flow due to buoyancy. It

is expected that the TKE dissipation rate estimates based on atmospheric measurements may also be biased due to these effects [7].

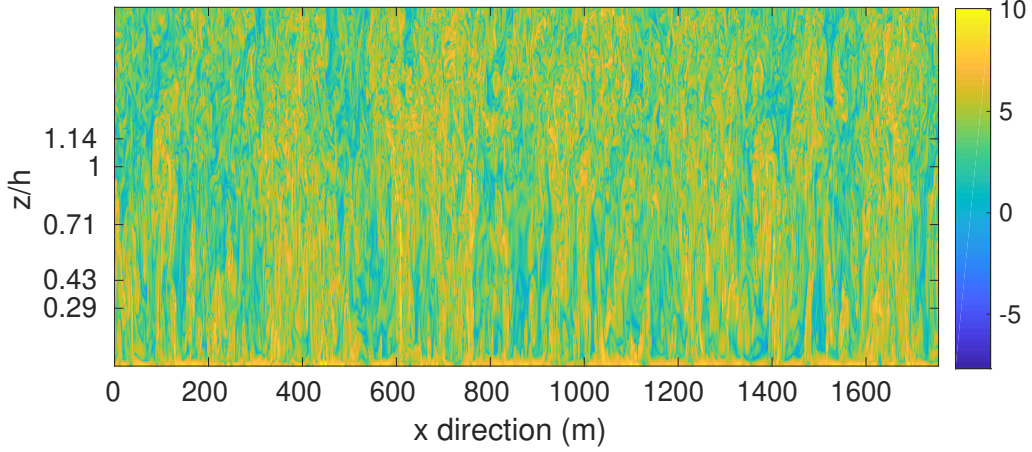


Figure 5.9: Vertical cross section of the logarithm of the enstrophy in the convective boundary layer showing horizontal plane $z = 0.29h, 0.43h, 0.71h, 1.0h, 1.14h$ where h is the CBL depth.

Table 5.3 presents values of ϵ , calculated with the power spectrum and the number of crossings, for horizontal plane $z = 1.0h$. ϵ_{PS} and ϵ_{NC} were estimated with the same procedure as in the first flow case. A large deviation from unity of the Λ/λ_n ratio, also in the core region of the flow, was observed. This could be caused by the same short-comings as in the previous case, i.e. low- Re number and external intermittency. In figure 5.13a, where k -fitting ranges were estimated from the velocity spectra, ϵ_{NC} agrees best with ϵ_{DNS} , in Fig. 5.13b, (k -fitting ranges resulting from D_2 function) all estimates are underpredicted in comparison to ϵ_{DNS} .

5.1.3 Moderate and low-resolution signals

Signals available from in situ airborne measurements are far from the idealized fully-resolved DNS data. Finite sampling frequency of a sensor and measurement errors induce effective spectral cutoffs of the velocity time series. In order to investigate the influence of the finite sampling on the TKE dissipation rate estimates, the following tests on the DNS data of stratocumulus cloud-top simulation are performed. A virtual aircraft that measures velocity signal with effective cut-off wavenumbers, $k_{cut} = 0.62, 1.25, 2.5, 5[m^{-1}]$, placed, approximately, within or close to the inertial range, is considered here. For each k_{cut} , if the aircraft flies in the streamwise x direction, a new path is created every 100 grid points in the y direction, such that 52

	k - fitting range	$\frac{\epsilon_{PS}}{B_0}$	$\frac{\epsilon_{NC}}{B_0}$	k - fitting range	$\frac{\epsilon_{PS}}{B_0}$	$\frac{\epsilon_{NC}}{B_0}$	$\frac{\epsilon_{D_2}}{B_0}$	$\frac{\epsilon_{D_3}}{B_0}$	$\frac{\epsilon_{SR}}{B_0}$	Λ/λ_n	$\frac{\epsilon_\lambda}{B_0}$
u in x	38 - 71	0.28	0.24	12-20	0.22	1.2	0.18	0.10	0.16	1.21	0.24
v in y	38 - 71	0.28	0.22	12-20	0.22	1.2	0.18	0.09	0.18	1.16	0.24
u in y	63 - 126	0.30	0.20	20-33	0.18	0.9	0.16		0.14	1.27	0.24
v in x	63 - 126	0.30	0.26	20-30	0.18	1.2	0.16		0.16	1.20	0.24
w in x	10 - 20	0.30	0.34	12-20	0.32		0.22		0.18	1.18	0.26
w in y	10 - 20	0.34	0.32	12-20	0.32		0.22		0.18	1.16	0.26

Table 5.3: Values of dissipation rate calculated using power spectrum and number of crossings for horizontal plane $z = 1.0h$. ϵ_{SR} , ϵ_λ , ϵ_{PS} , ϵ_{NC} , ϵ_{D_2} and ϵ_{D_3} are the dissipation rates calculated from Eqs. (3.10,3.11), Eq. (3.2), Eq. (3.18), Eq. (3.20) and Eqs. (3.19), respectively. $\epsilon_{DNS}/B_0 = 0.26$ and Λ/λ_n is the ratio of zero crossing micro-scale to the Taylor's micro-scale. The first fitting ranges seemed optimal for power spectra, the second - for structure functions.

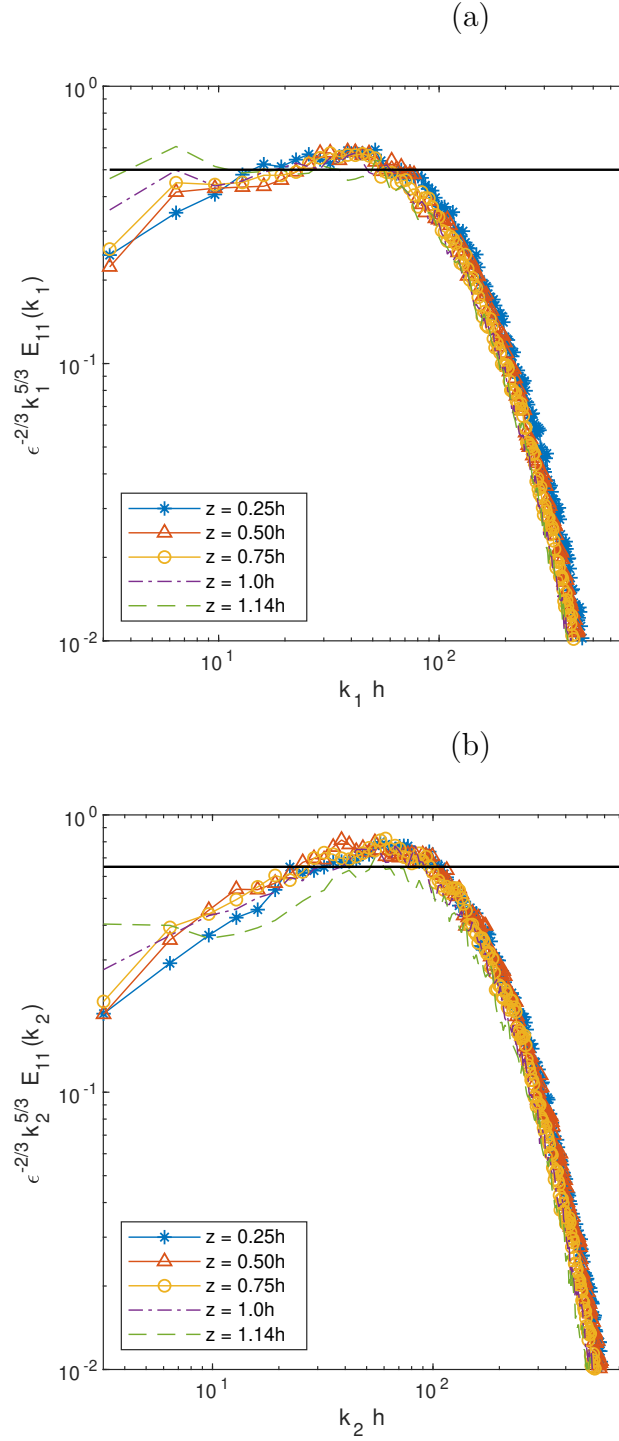


Figure 5.10: Convective boundary layer simulation. Compensated 1D velocity spectra of the u velocity component at $z \in \{0.29h, 0.43h, 0.71h, 1.0h, 1.14h\}$ a) longitudinal, b) transverse.

signals are collected. Similarly, if the aircraft flies in the y direction, 52 paths in x direction is created. In the first test, the obtained power spectra and $\langle u_i'^2 \rangle N_i^2$ profiles

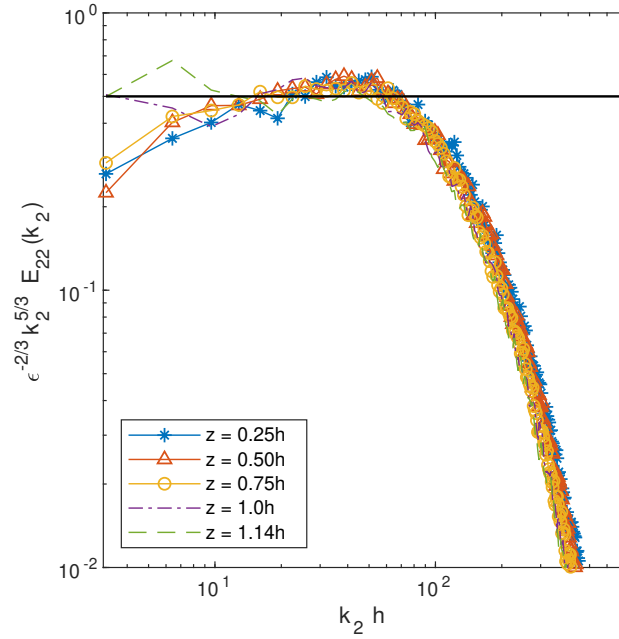
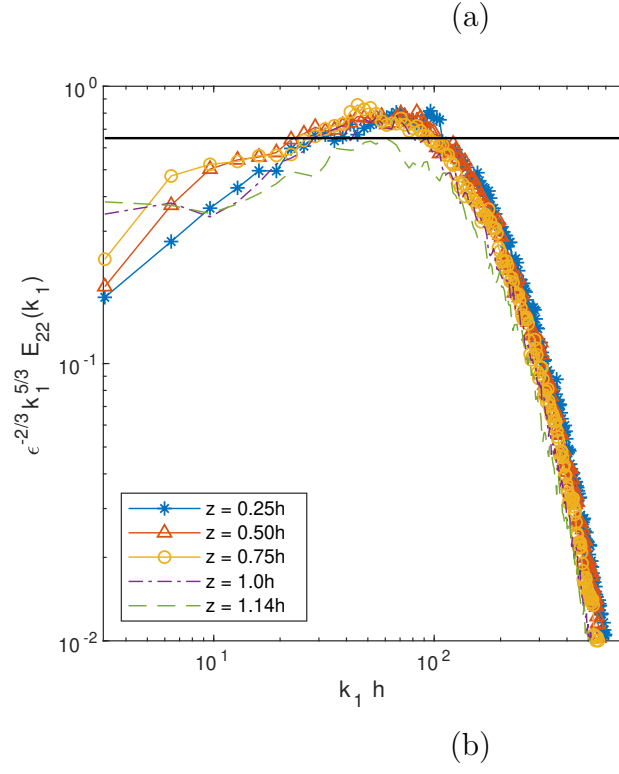


Figure 5.11: Convective boundary layer simulation. Compensated 1D velocity spectra of the v velocity component at $z \in \{0.29h, 0.43h, 0.71h, 1.0h, 1.14h\}$ a) transverse, b) longitudinal.

are averaged and TKE dissipation rates ϵ_{PS} and ϵ_{NC} are calculated. Finite sampling frequency cause aliasing i.e. spectral densities for k higher than the wavenumber k_{cut}

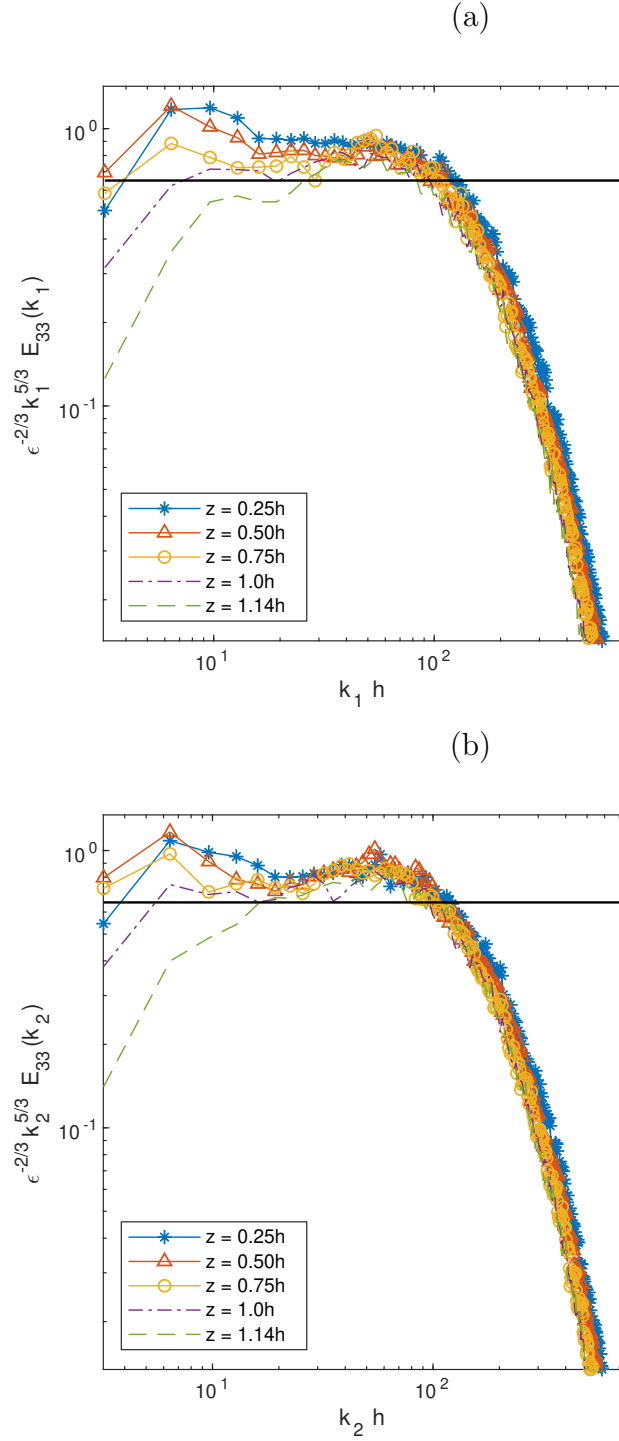


Figure 5.12: Convective boundary layer simulation. Compensated 1D velocity spectra of the w velocity component at $z \in \{0.29h, 0.43h, 0.71h, 1.0h, 1.14h\}$ a) transverse in x direction, b) transverse in y direction.

are added to the spectral densities at $k < k_{cut}$. This causes a bias error of the TKE dissipation rate estimates. As seen in Fig. 5.14, the bias of ϵ_{NC} is smaller than the

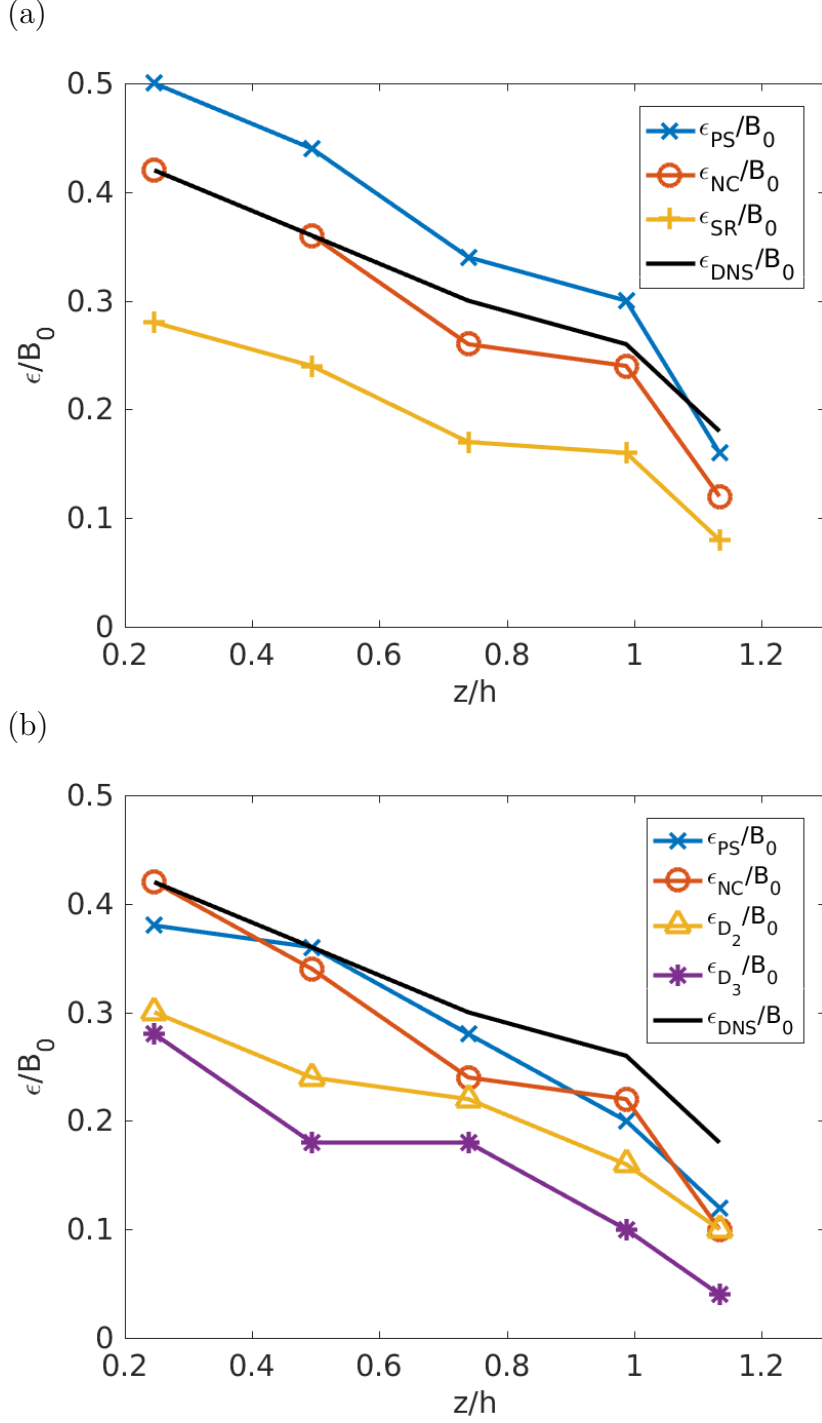


Figure 5.13: TKE dissipation rate of free convective boundary layer simulation calculated from Eq. (3.18), Eq. (3.20) and Eqs. (3.10), (3.11), (a) Fitting ranges were estimated based on E_{11} and E_{22} functions, (b) Fitting ranges were estimated based on D_2 .

bias of ϵ_{PS} . In particular, results of ϵ_{NC} for $k_{cut} = 1.25[m^{-1}]$ are still close to ϵ_{DNS} . This result is in line with the error analyses performed in Ref. [144] on artificially

generated velocity time series where a smaller bias error, however somewhat larger scatter of ϵ_{NC} was observed in comparison to ϵ_{PS} . In the present analysis, no additional corrections is introduced, neither to the power spectra, nor to the $\langle u_i'^2 \rangle N_i^2$ profiles, to reduce the bias (such methods can be formulated for high- Re flows, see [124]).

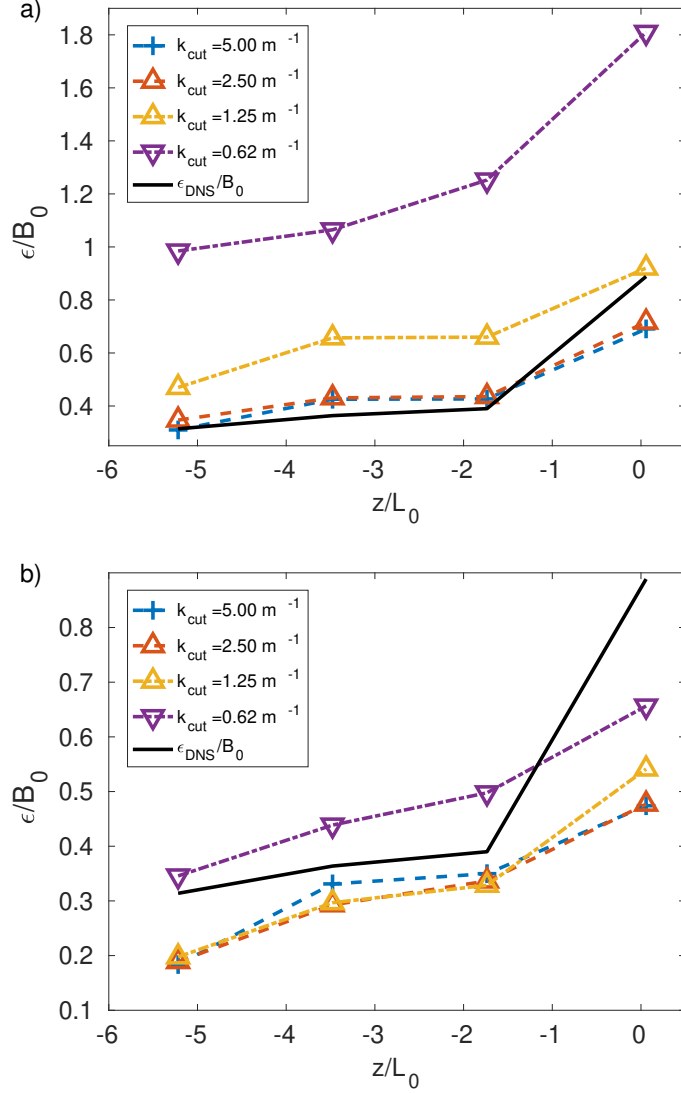


Figure 5.14: Normalized TKE dissipation rate estimates from signals with effective cut-off's k_{cut} as a function of vertical coordinate z/L_0 (dimensionless) a) ϵ_{PS} , b) ϵ_{NC} .

Next, in order to perform a scatter test of the results, I estimate ϵ_{PS} and ϵ_{NC} from each velocity signal, separately. For all signals, the same fitting range, $k = [0.29 \text{ m}^{-1}, 0.58 \text{ m}^{-1}]$ is used. In Fig. 5.15, I plot ϵ_{PS} vs. ϵ_{NC} calculated at the plane $z = -5.2L_0$ for $k_{cut} = 5[\text{m}^{-1}]$ and $k_{cut} = 0.62[\text{m}^{-1}]$. In Fig. 5.15a, larger scatter

of ϵ_{NC} is observed, however, as k_{cut} decreases, scatter of both ϵ_{NC} and ϵ_{PS} becomes comparable, see Fig. 5.15b. In Fig. 5.16, the r.m.s. of ϵ_{NC} and ϵ_{PS} estimates at plane $z = -5.2L_0$ are plotted. A moderate increase of r.m.s. of ϵ_{NC} and much larger change of ϵ_{PS} for $k_{cut} = 0.62m^{-1}$ are observed. The obtained result confirm the method based on the number of crossings respond differently to errors due to finite sampling, than the spectral retrieval technique.

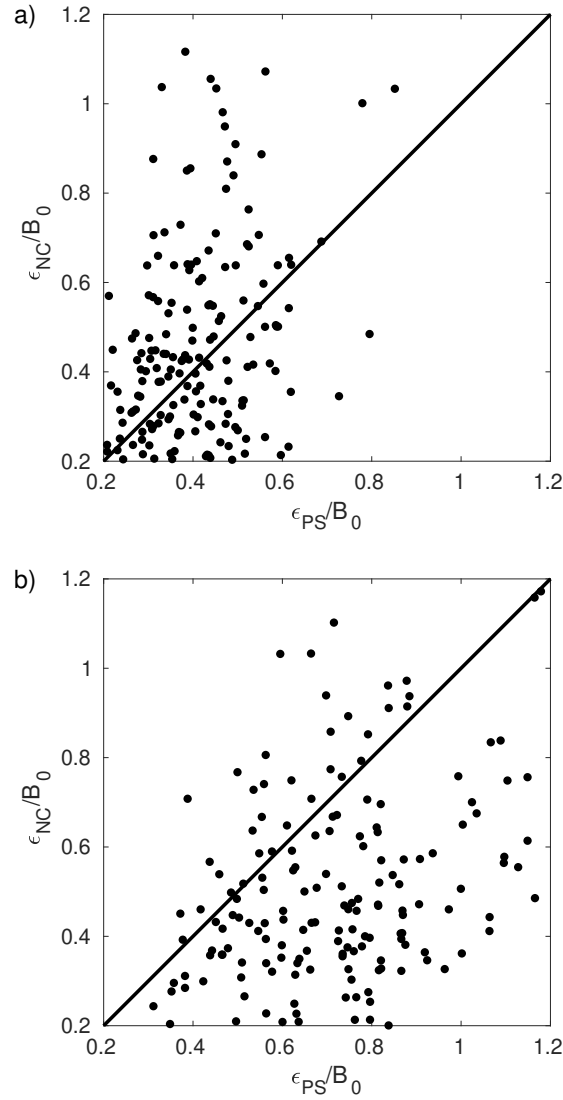


Figure 5.15: Results of ϵ_{NC} vs. ϵ_{PS} normalised with B_0 for signals with a) $k_{cut} = 5[m^{-1}]$ b) $k_{cut} = 0.62[m^{-1}]$.

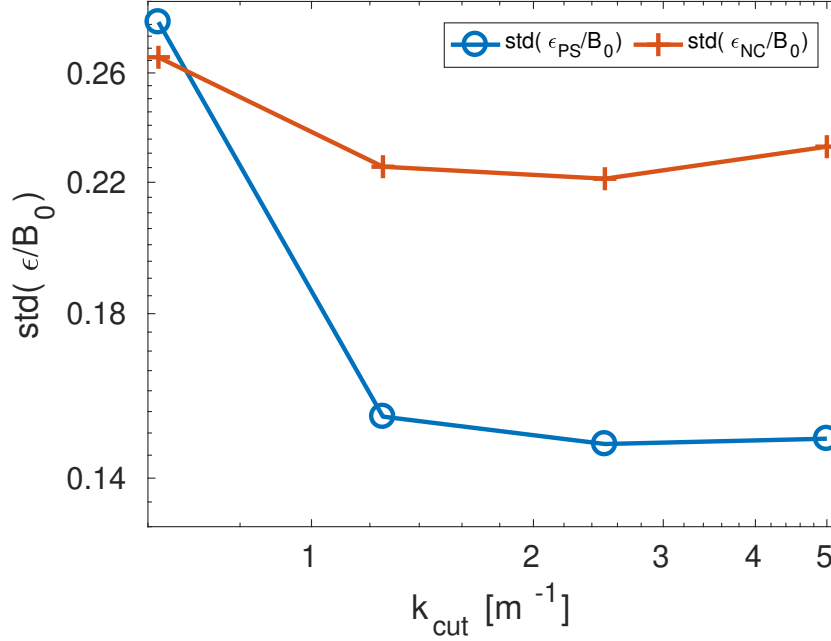


Figure 5.16: Standard deviations of ϵ_{NC} and ϵ_{PS} estimates normalized with B_0 as a function cut-off k_{cut} .

5.2 TKE dissipation rate estimation with the direct and iterative methods

Results discussed in Section 5.1 show that the TKE dissipation rate recovery based on inertial-range arguments is difficult in the considered cases. First source of error is due to the relatively low- Re of DNS simulations. Although inertial ranges of atmospheric high- Re flows cover a few decades of k numbers, finite averaging windows and finite resolutions of the measurements cause analogous problems - results are in fact dependent on the chosen fitting ranges. Moreover, dissipation rate estimates are biased due to buoyancy effects.

In this section, the estimation of ϵ with direct and iterative methods is discussed. There are still discrepancies between ϵ estimate using the iterative methods and ϵ_{DNS} caused by the deviation of Λ/λ_n different from unity. It is also shown that the ratio Λ/λ_n can be used as a measure of external intermittency. The new formulation of the iterative methods discussed in section 3.4 will be analyzed.

5.2.1 Direct methods

The dissipation rate ϵ_{SR} was estimated from the Sreenivasan-Rice formulae Eqs. (3.10) and (3.11) [130]. In Table 5.1, results of direct methods are presented. ϵ_{SR} from the Sreenivasan and Rice formula based on the number of crossings, Eqs. (3.10 and 3.11) and ϵ_λ based on the Taylor's microscale from Eq. (3.2) were calculated. The discrepancy between ϵ_{SR} obtained with Sreenivasan et al's formula Eqs. (3.10) and (3.11) and ϵ_λ is caused by the Λ/λ_n values which deviate from unity. This could be caused by the low- Re number of the considered flow, its physical complexity and, in particular, strong non-Gaussianity of the PDF's of velocity derivatives. The estimates of ϵ_λ given in Table 5.1 are identical for velocity components u and v , both for the longitudinal and transverse direction and are close to $\epsilon_{DNS} = 0.36B_0$, while estimates from the vertical component are somewhat over-predicted. Still, it can be concluded that at this layer, at small scales, the local isotropy assumption for the calculation of ϵ is well satisfied. Although ϵ_{NC} is also calculated from the number of crossings, its estimates are closer to ϵ_{DNS} than the corresponding estimates ϵ_{SR} . The reason is that Λ/λ_n changes additionally with k_{cut} for the filtered signals and, after filtering out the smallest scales, is closer to unity. In Table 5.3, ϵ_{SR} are underestimated due to the same reasons discussed above. Estimates from the vertical velocity component w differ from the remaining estimates.

5.2.2 Iterative method

In this section, the second approach from Ref. [144], is considered, as described in Section 3.3, where the cut-off can be moved towards dissipative part of the spectrum. First, an optimal model for the function f_η in Eq. (3.24) should be chosen, be it the Pope (3.15), Pao (3.17) or the exponential model (3.16). Figure 5.17 shows model spectrum of u in x for horizontal plane $z = -3.5L_0$ of the cloud-top simulation with different formulations of f_η . The Pope formulation provides much better fit with DNS than the Pao or exponential models, both for the longitudinal and transverse spectra (see figure 5.17). The same is observed in the free convective boundary layer flow case, see Fig. 5.18. Hence, in the remaining part of this section, all predictions will be made with the Pope model for f_η , as given in Eq. (3.15).

The DNS signal being investigated is first low-pass filtered with the use of 6th order Butterworth filter with a given k_{cut} . I will investigate how accurate are the predictions of the TKE dissipation rate from the filtered signal and how they depend on k_{cut} . According to the procedure described in Ref. [144], in order to estimate ϵ , a

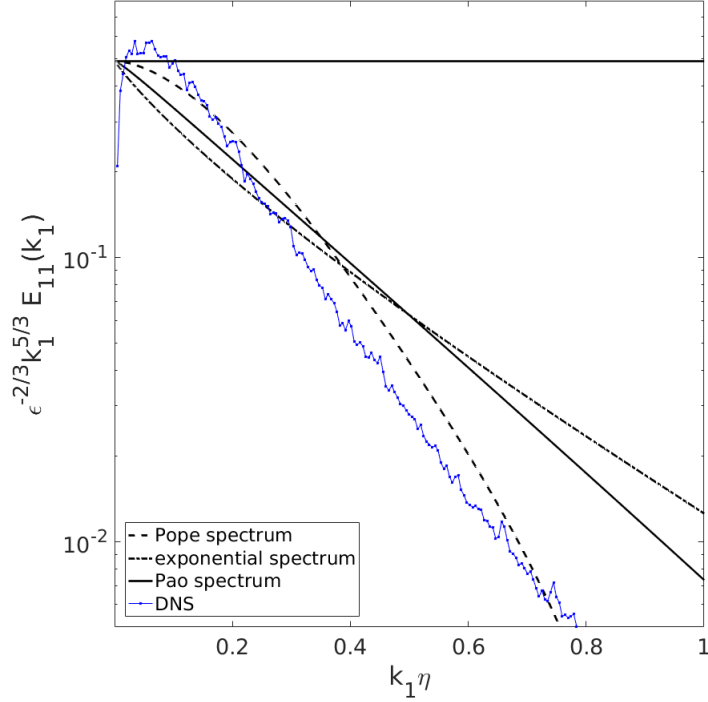


Figure 5.17: Stratocumulus cloud top simulation. Model spectrum of u in x at $z = -3.5L_0$ with dissipative ranges described by Eqs. (3.15), (3.17), (3.16).

first guess for the Kolmogorov length $\eta = (\nu^3/\epsilon)^{1/4}$ is made. One can take $\epsilon^0 = \epsilon_{PS}$, however, independently of the initial guess, the procedure always converges to the same value of ϵ_{NCR} (see [144]). The correcting factor is calculated from Eq. (3.24) and next, the value of dissipation rate is estimated with Eq. (3.25). The integrals in Eq. (3.24) is approximated with the trapezoidal rule. The procedure is repeated as described in section 3.3 until the condition $\Delta\eta = |\eta^{n+1} - \eta^n| \leq d_\eta$ with $d_\eta = 10^{-8}$ is satisfied. Convergence is reached in all simulation before the 10th iteration.

Figure 5.19a shows ratios $\epsilon_{NCR}/\epsilon_{DNS}$ for different cut-off wavenumbers for the cloud top simulations. First, the case where k_{cut} is placed within the inertial range is investigated. k_2 and k_1 are, respectively, the upper and lower end of this range. As it is seen, results depend on k_{cut} , due to deviations from Kolmogorov scaling and the fact that Rice formula (3.4) is only approximately satisfied for the considered signals. Let us define the length scale of the filtered signal, analogous to the Taylor microscale (3.3) λ_{cut}

$$\lambda_{cut} = \frac{1}{\sqrt{2}} \left[\frac{2\langle u_{cut}^{\prime 2} \rangle}{\langle (\partial u_{cut}' / \partial x)^2 \rangle} \right]^{1/2}. \quad (5.1)$$

Analogously, $\Lambda_{cut} = 1/(\pi N_{cut})$ will denote Liepmann scale calculated for the filtered

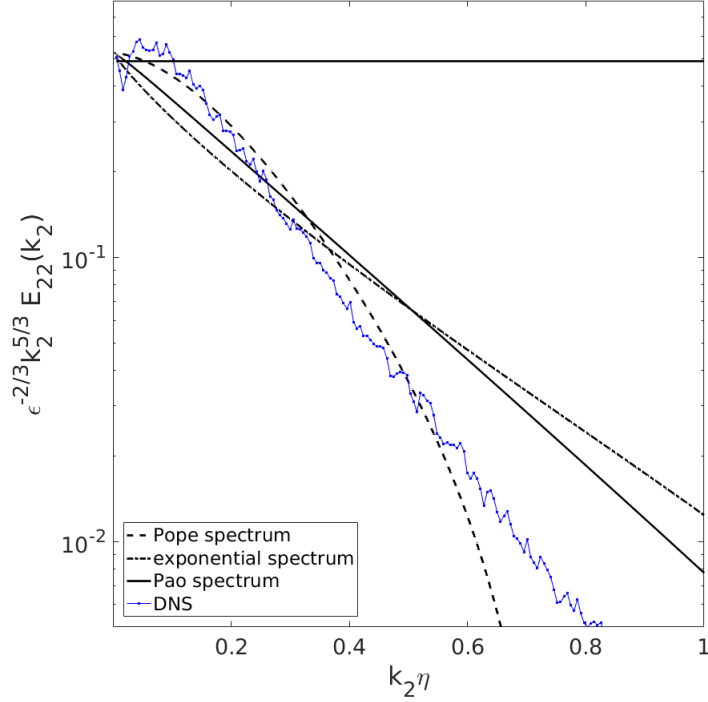


Figure 5.18: Free convective boundary layer simulation. Model spectrum of v in y at $z = 1.0h$ with dissipative ranges described by Eqs. (3.15), (3.17), (3.16).

signal. In the case of the airborne measurements of high- Re turbulence investigated in Ref. [144], the condition $\Lambda_{cut}/\lambda_{cut} \approx 1$ was satisfied with a good accuracy. Therein, the cut-off wavenumber was placed in the inertial range. As far as the present DNS data are concerned, $\Lambda_{cut}/\lambda_{cut}$ changes with k_{cut} (results not shown here). It is closer to 1 if k_{cut} is placed in the inertial range, however, increases with increasing k_{cut} towards values presented in Tables 5.1-5.3.

In Fig. 5.19b, results of ϵ_{NCR} averaged over all k_{cut} from the inertial range is showed. It is seen that ϵ_{NCR} estimates are very close to DNS with about 6% difference (excluding $z = 0.1L_0$ horizontal plane). It will be shown later that the discrepancies in these results are due to high external / global intermittency which is a setback for the number of crossings approach when applied to complex flows. In the core region, results are better than ϵ_{NC} calculated in section 5.1.1. It seems that ϵ_{NCR} is in fact influenced by the chosen form of f_η irrespective of the fitting range, hence, the results are improved when a model for f_η is taken into account.

Figure 5.20 presents the same results as described above, but for the free CBL case. Here, we observe larger discrepancies between ϵ_{NCR} and ϵ_{DNS} .

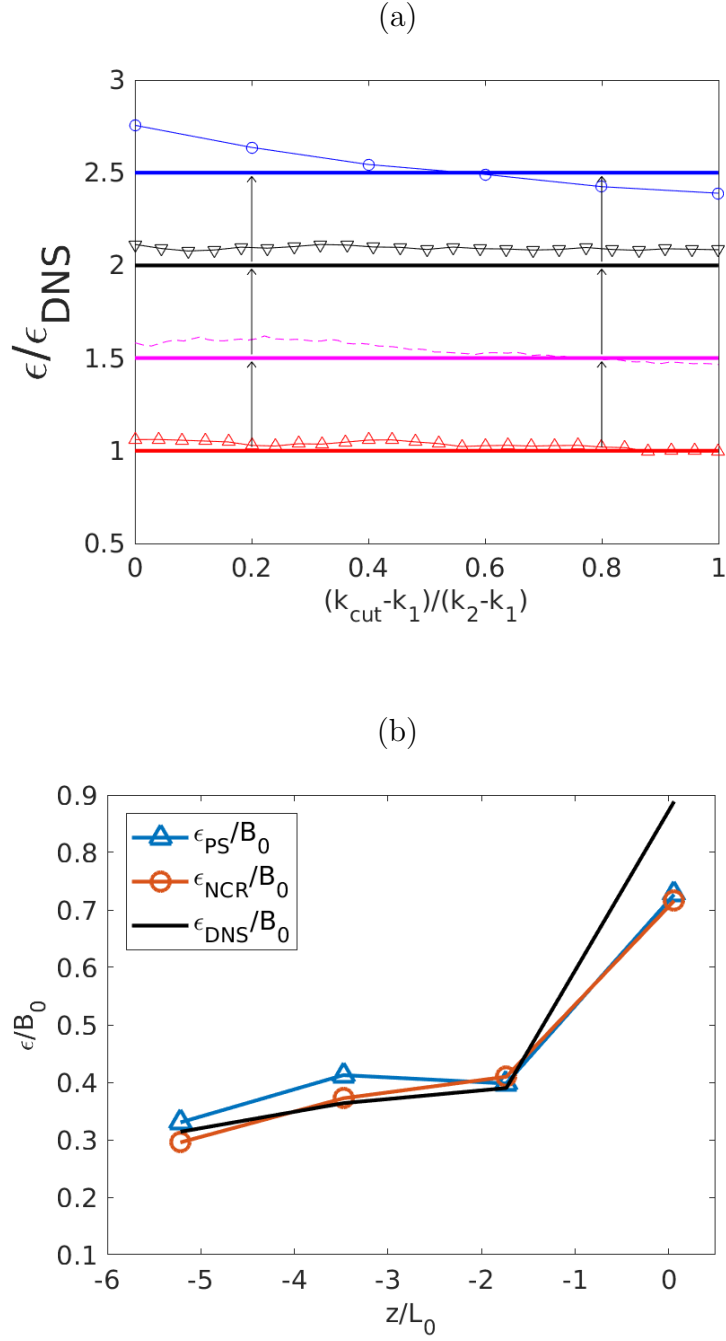


Figure 5.19: a) TKE dissipation rate estimate from Eq. (3.25) as a function of cut-off wavenumber k_{cut} compared with with DNS dissipation rate value (thick lines) for different horizontal planes of cloud top simulation. Rows from top to bottom are $z = 0.1L_0$ (blue - circle), $z = -1.7L_0$ (black - down pointed triangle), $z = -3.5L_0$ (magenta - dash) and $z = -5.2L_0$ (red - triangle). Different plots are moved by a constant number 0.5 for better visibility. b) TKE dissipation rate estimates from Eq. (3.18) and Eq. (3.25) compared with DNS with k_{cut} placed in the inertial range

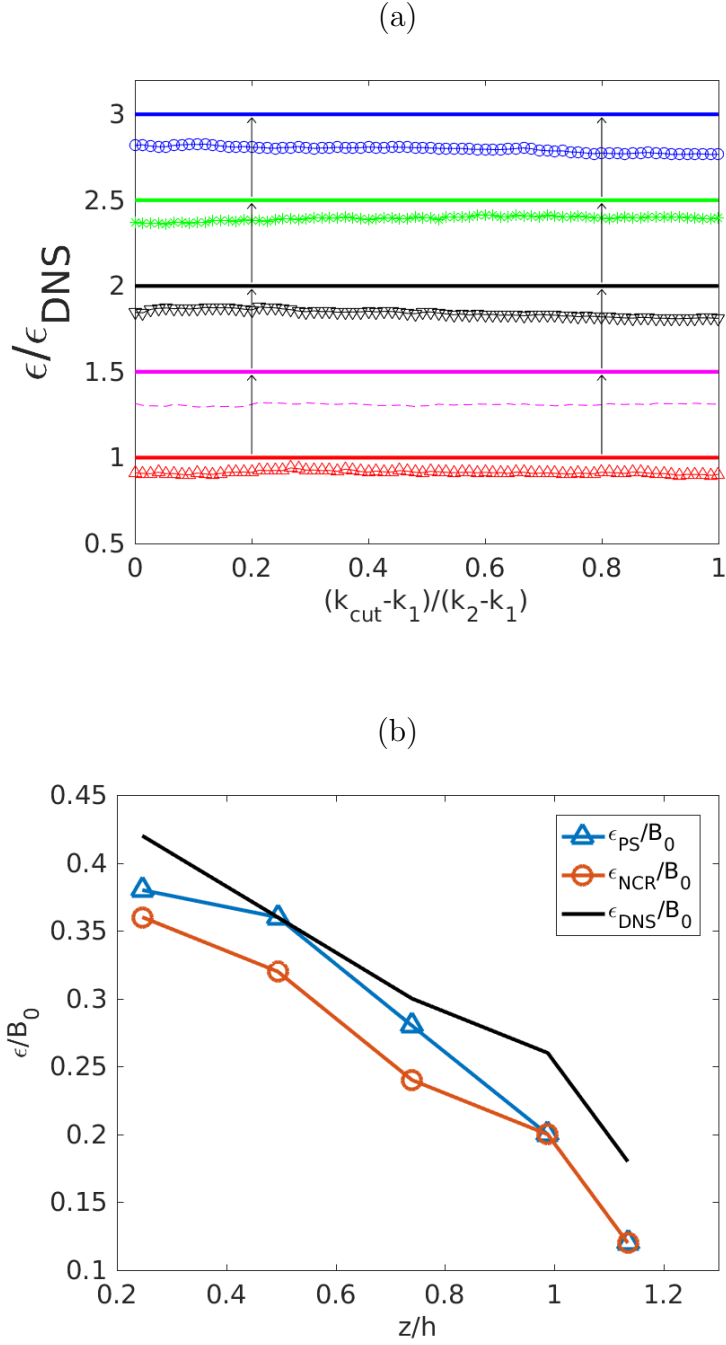


Figure 5.20: a) TKE dissipation rate estimate from Eq. (3.25) as a function of cut-off wavenumber k_{cut} compared with with DNS dissipation rate value (thick lines) for different horizontal planes of free convective boundary layer simulation. Rows from top to bottom are $z = 1.14h$ (blue circle), $z = 1.0h$ (green - star), $z = 0.71h$ (black - down pointed triangle), $z = 0.43h$ (magenta - dash) and $z = 0.29h$ (red - triangle). b) TKE dissipation rate estimates from Eq. (3.18) and Eq. (3.25) compared with DNS with k_{cut} placed in the inertial range

In both flow cases, the results are deteriorated once k_{cut} increases, this is caused by the increase of $\Lambda_{cut}/\lambda_{cut}$ values. The influence of this ratio on results is investigated in the following section. Next, in order to improve the results, in section 5.2.4, analysis with the new, modified proposal put forward in section 3.4 will be performed.

5.2.3 Λ/λ_n ratio as the intermittency measure

Due to the observed changes of Λ/λ_n ratio in the vertical direction for both flow cases, another idea developed within this work is to use the Taylor-to-Liepmann scale as an indicator of external intermittency γ .

In the literature, several methods were proposed to differentiate between rotational (turbulent) and irrotational (non-turbulent) parts of a measured velocity signal [156]. Each of them requires definition of an indicator function q , a criterion function $f(q)$ and a threshold level T_h . The flow is assumed turbulent when $f(q) > T_h$. In case instantaneous values of vorticity $\boldsymbol{\omega} = \nabla \times \mathbf{u}$ are known from measurements or DNS data, the enstrophy

$$\Omega = 1/2|\boldsymbol{\omega}|^2 \quad (5.2)$$

can be used as the criterion function $f(q)$. However, γ estimation based on vorticity may also be subject to error due to presence of mean gradients or non-turbulent wave-like motions which spuriously increase Ω above the threshold. As a remedy, a generalized conditioning method based on the vorticity of high-pass filtered velocity fields was proposed in Ref. [11].

In this work, γ calculated based on enstrophy is compared to the Taylor-to-Liepmann scale ratio. As a first approximation, it is assumed that in the externally intermittent flow, the statistics will change to $\gamma\langle u'^2 \rangle$ and $\gamma\langle (\partial u'/\partial x)^2 \rangle$. Moreover, the laminar part of the signal does not significantly contribute to the number of crossings, hence γN_L crossings per unit length in the intermittent signal will be detected. With this, the Taylor microscale, the Liepmann scale and their ratio will change to

$$\lambda_{nI} = \left[\frac{\gamma\langle u'^2 \rangle}{\gamma\langle (\partial u'/\partial x)^2 \rangle} \right]^{1/2} = \lambda_I, \quad \Lambda_I = \frac{1}{\gamma\pi N_L} = \frac{1}{\gamma}\Lambda, \quad \frac{\lambda_{nI}}{\Lambda_I} = \gamma \frac{\lambda_n}{\Lambda}, \quad (5.3)$$

where the subscript I is related to the statistics in the intermittent flow. If $\lambda_n/\Lambda \approx 1$, then in the intermittent flow, $\lambda_{nI}/\Lambda_I \approx \gamma$. The following part of this work is intended to improve the predictions of TKE dissipation rate with the iterative method. However, in this case, λ_n/Λ is around 0.8 even in the core region of the flow. Predictions

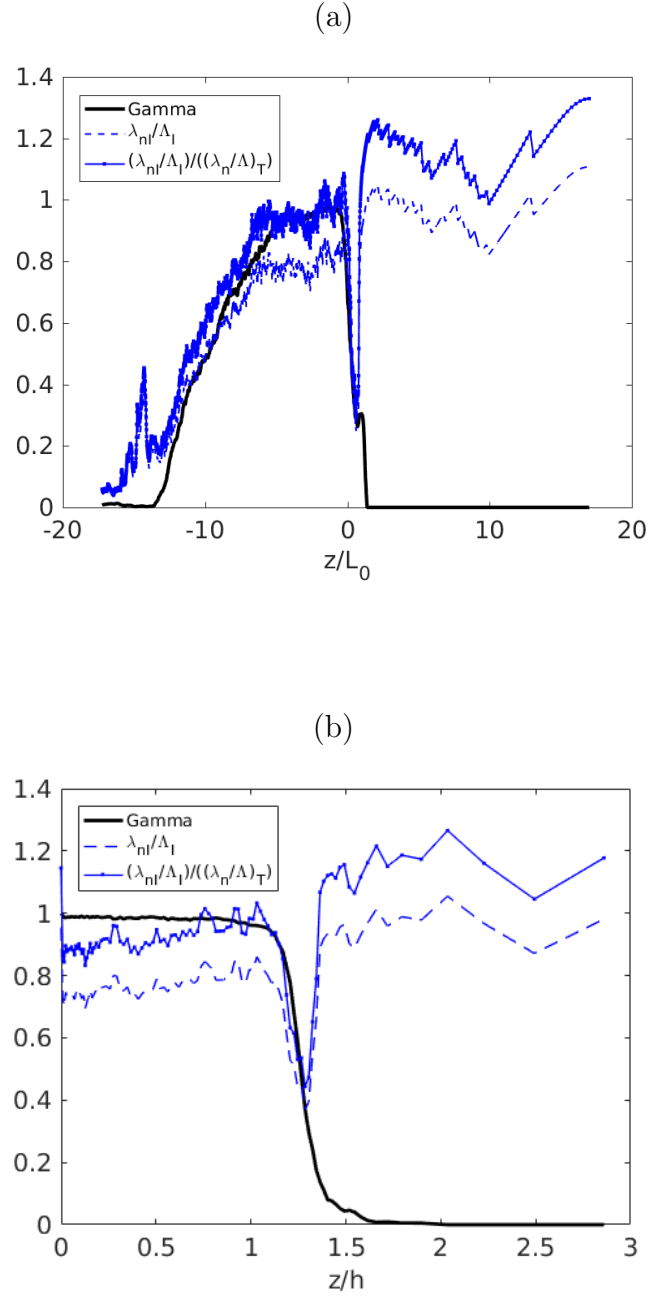


Figure 5.21: Values of the intermittency factor calculated from the enstrophy and λ_n/Λ . a) stratocumulus cloud top, b) convective boundary layer.

of Eq. (5.3), i.e. the ratio

$$\frac{\lambda_{nI}/\Lambda_I}{(\lambda_n/\Lambda)_T} \approx \gamma \quad (5.4)$$

(the subscripts T is used to denote mean value in the turbulent, core region of the flow) were compared with γ estimated using the well-established method based on the instantaneous enstrophy Ω [11]. For this, profiles of γ in the vertical direction were

calculated. Regions where Ω was smaller than a certain threshold value were identified as "laminar spots". Results of γ were averaged in the streamwise direction for a given plane, and, additionally in the spanwise direction over four planes $x/L_0 = 0, 13.5, 27$ and 40.5 in the stratocumulus cloud-top simulations and $x/L_0 = 0, 54, 108$ and 162 in the free convective boundary layer case. In Fig. 5.21, these profiles were compared with calculated ratio from Eq. (5.4). $(\lambda_n/\Lambda)_T = 0.83$ is taken for the stratocumulus cloud top and free convection.

Favourable agreement between both curves at least for larger γ values were observed. Discrepancies for small γ are due to numerical errors, as both Λ and λ_n are small in these regions. This result also agrees with the work of Nzotungishaka [94]. He found a good agreement between predefined intermittency ratio γ of artificial signals with its Taylor-to-Liepmann ratio. Hence, Taylor-to-Liepmann ratio can be used as a measure of external intermittency.

5.2.4 New formulation for the iterative approach

As observed in the two flow cases analyzed above, the Λ/λ_n value is different from unity, even in the turbulent, core region of the flow. This fact is the source of existing discrepancies between ϵ_{NCR} and ϵ_{DNS} . The deviations of Λ/λ_n from unity could be caused by the strong non-Gaussianity of the velocity derivative (related to the phenomenon of internal intermittency) and external or global intermittency connected with the existence of laminar spots within the turbulent flow.

To overcome these problems, the new, modified approach for ϵ retrieval was proposed in section 3.4. Instead of the number of crossings per unit length, it is proposed to use the variance of velocity derivative. The procedure for this new formulation is almost the same as in the second approach from Ref. [144], see Eq. (3.25). Again, the first value of η is guessed, next the correcting factor $\mathcal{C}_{\mathcal{F}}$ is computed from Eq. (3.24) and the value of dissipation is estimated with Eq. (3.29). The next iteration starts by calculating again the Kolmogorov length $\eta = (\nu^3/\epsilon)^{1/4}$ with the new $\epsilon_{\lambda R}$, the corrected value of $\mathcal{C}_{\mathcal{F}}$ from Eq. (3.24) and the new value of $\epsilon_{\lambda R}$ from Eq. (3.29). Again, after several iterations, the procedure converges to the final values of the dissipation rate and Kolmogorov's length η within a prescribed accuracy. The function f_η with the exponential Eq. (3.16), Pao Eq. (3.17) and Pope Eq. (3.15) formulas were used to model the dissipative range of the stratocumulus cloud top simulation and free convective boundary layer data. ϵ for different values of cut-off wavenumber k_{cut} is estimated, starting from the lower-end of the inertial range to the upper-end of the dissipative range.

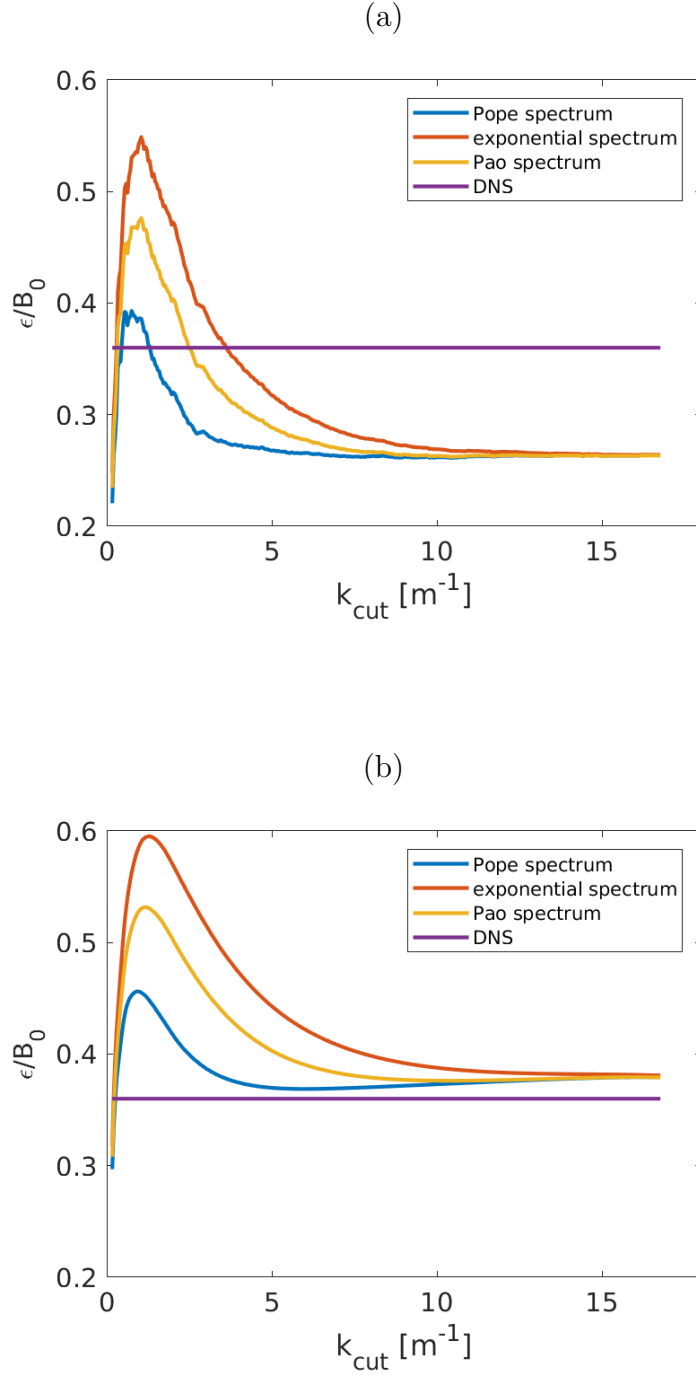


Figure 5.22: The plot of ϵ estimate against different k_{cut} . Results for u in x signal and for plane $z = -3.5L_0$ of the stratocumulus cloud-top simulation. a) method based on the number of crossings and Eq. (3.25) b) new formulation, Eq. (3.29). The straight magenta line represent the value of ϵ_{DNS} .

In figure 5.22 and 5.23, estimates from the number of crossings ($\langle u'^2 \rangle N_{cut}^2$), Eq. (3.25) and the new proposal, Eq. (3.29) for both considered flow cases are presented.

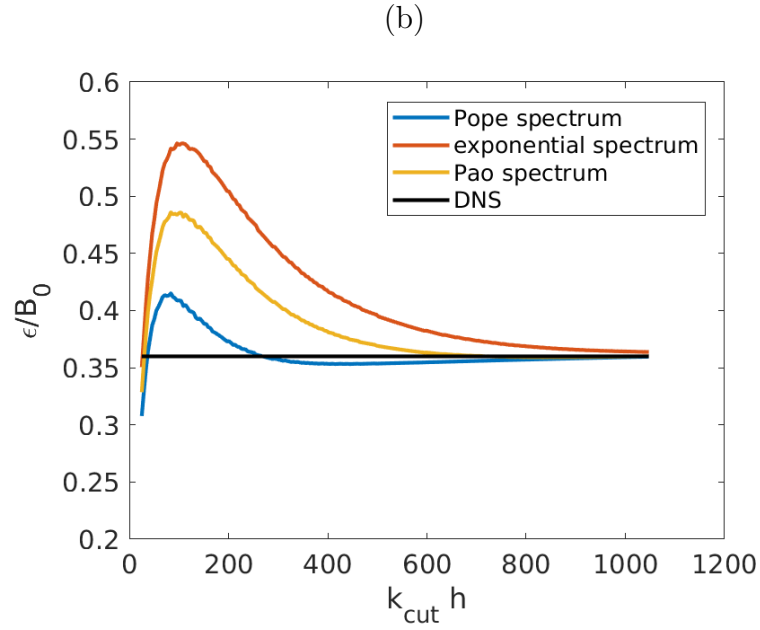
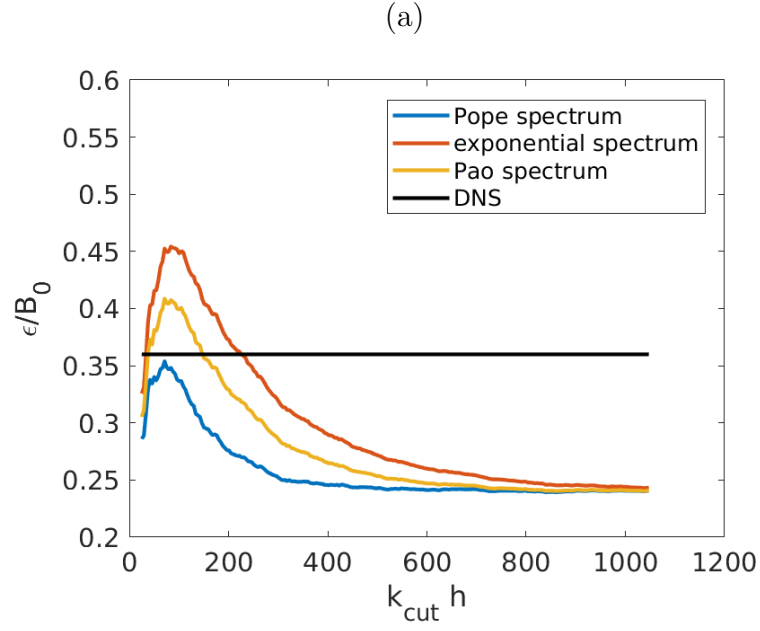


Figure 5.23: The plot of ϵ estimate against different k_{cut} . Results for u in x signal and for plane $z = 0.43h$ of the free convective boundary layer case. a) method based on the number of crossings and Eq. (3.25) b) new formulation, Eq. (3.29). The straight magenta line represent the value of ϵ_{DNS} .

Results of the new formulation, shown in Figs. 5.22b and 5.23b compare favourably with DNS over wide range of k_{cut} numbers. In figure 5.22a, wavenumbers k_{cut} from the

inertial range agree better with DNS (similar to what we observe in figure 5.19) but as k_{cut} increases towards the dissipative range, ϵ_{NCR} value for the three model spectra f_η , converge to the same, under-predicted value. In figure 5.22b, at wavenumber k_{cut} from the dissipative range, the estimated $\epsilon_{\lambda R}$ compare favourably with ϵ_{DNS} . In both figures 5.22 and 5.23, the best estimates, over a large range of k_{cut} are observed for the Pope model.

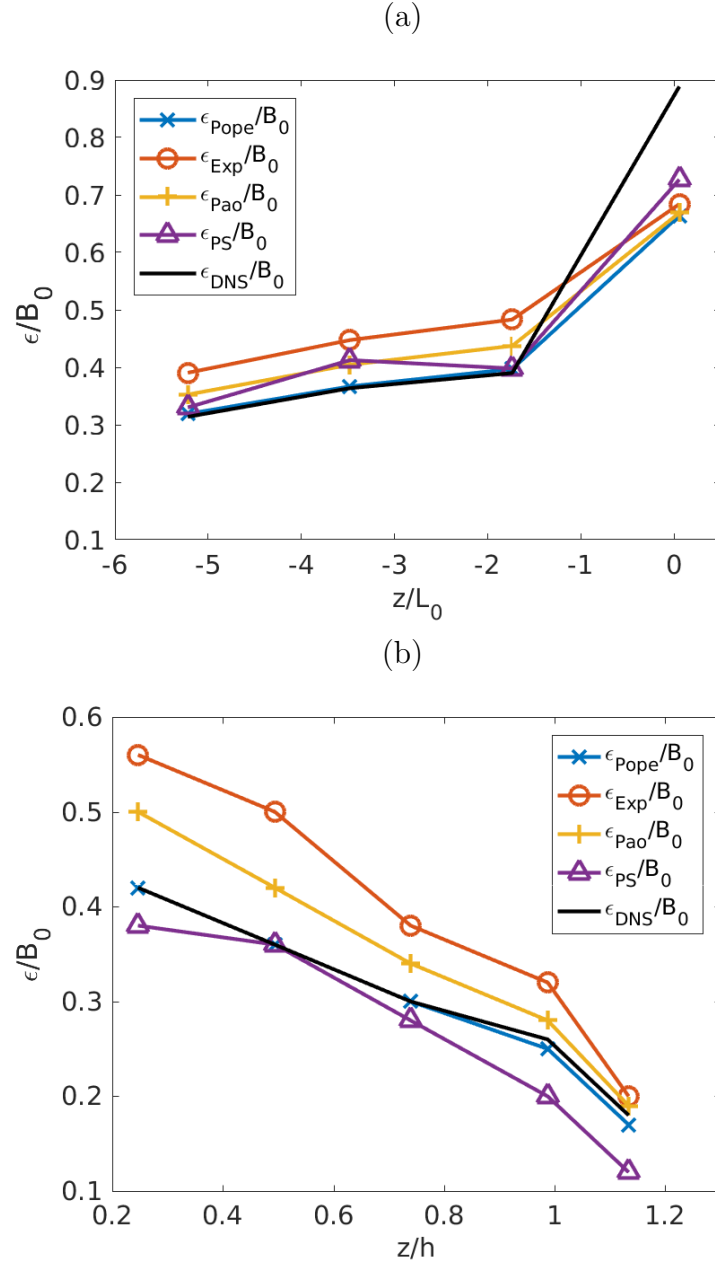


Figure 5.24: The plot of ϵ estimate with different model spectrum for different horizontal profiles a) for cloud top simulation flow case. b) for free convective boundary layer flow case.

Figure 5.24 shows $\epsilon_{\lambda R}$ estimates using the new formulation (3.29) with different model spectra f_η for different horizontal profiles of the two flow cases. Figure 5.24a shows ϵ estimates for the stratocumulus cloud top simulation flow case. This ϵ estimates were calculated at $k_{cut} = 5.3m^{-1}$, which is within the dissipative range. It is observed that the Pope model spectrum with the new formulation predicts ϵ_{DNS} well for all horizontal profiles (except at the horizontal profile $z = 0.1L_0$ that is strongly affected by stable stratification and shear). For the free convective boundary layer flow case reported in figure 5.24b, all ϵ estimates were calculated at $k_{cut}h = 614$. It is observed that the Pope model spectrum with the new formulation predicts ϵ_{DNS} well for all horizontal profiles. This shows that the new formulation with Pope's model for dissipative range of the spectrum f_η can predict ϵ for complex flows better than the number of crossings method. As it was argued, the reason for the discrepancies are the deviations of Λ/λ_n from unity.

Part 2

Numerical reconstruction of small-scale turbulence

Chapter 6

Fractal reconstruction of small scales in large eddy simulation

6.1 Introduction

In part 1, various retrieval methods used for estimating turbulence kinetic energy dissipation rate ϵ were discussed. The quantity ϵ can be used to describe small-scale turbulence in a statistical sense. Moreover, as predicted by the Kolmogorov's second similarity hypothesis, ϵ determines the energy spectrum in its self-similar, inertial part. In part 2, the focus is on this self-similarity property of turbulent motions in this range of scales. It will be used to reconstruct the small scales from the high-wavenumber part of the energy spectrum. This is important because small scales play crucial role in predicting complex processes such as cloud/rain formation, pollutant dispersion, sediment transport in water bodies, fibre suspension and spray combustion, to mention a few. These processes can best be studied using DNS, since it resolves all turbulent scales needed for the time evolution of such processes [37]. As mentioned in chapter 4, this simulation approach poses unrealistic computational cost at high Reynolds numbers. LES provides a compromise, in which the large scale features of the flow are fully resolved while sub-grid (unresolved) scales are modelled. For instance, LES prediction of particle trajectories in turbulent flows requires a good sub-grid scale model. Sub-grid scale model errors can lead to the progressive divergence of particle trajectories when compared with those obtained in experiment or DNS [79, 80]. As a result of these errors, particle statistics such as preferential concentration, average settling velocity and relative velocities are either over- or under-estimated [15, 67, 91, 109, 129, 137, 155].

6.2 State of the art

Several attempts have been made to develop models for the effects of sub-grid scales of turbulence, especially on the prediction of the Lagrangian dispersion of inertial particles [79, 106, 116, 117]. As classified by Ref. [79], there are stochastic and structural models. Stochastic models (also called functional models [53]) are based on the solutions of the Langevin equations [32, 106, 108] supplemented with a stochastic Wiener process term [24, 50]. They are aimed at retrieving only some statistical properties of the sub-grid velocity field. Various works on stochastic models show that they perform well at small Stokes number but have strong sensitivity to filter size [28, 79].

Structural sub-grid models are an alternative to the stochastic models and they aim at reconstructing some of the features of the subgrid velocity field. These models allow for the approximate reconstruction of two-point particle statistics at the subgrid scales [92, 129, 137]. Examples of structural models are the fractal interpolation [5, 6, 17, 80, 120], approximate deconvolution (ADM) [44, 88, 136, 157], spectrally optimized interpolation [45] and the kinematic simulations based on Fourier modes [40, 76, 77, 107].

A good structural sub-grid scale reconstruction model should not only be able to capture the statistics of small scales but also be computationally efficient and easy to use. Fractal interpolation technique (FIT) seems promising (especially for high Re geophysical applications) with respect to these features. The word *fractal* is a pattern that repeats itself at different scales, called self-similarity. This pattern is seen in nature, especially in turbulent motion of fluids. As a result, the focus is on the application of this fractal technique to turbulence. FIT can be used to parameterize sub-grid scale stresses [120]. It also includes the correlations of subgrid scales with large scale field, which are necessary for sufficient energy transfer to take place. FIT was introduced to construct synthetic, fractal subgrid-scale fields applied to LES of both steady and freely decaying isotropic turbulence [120]. The underlying assumption of the model is the existence of fractal-scale similarity of velocity fields. This assumption can be sufficiently valid only within the inertial-range scales. An attribute of the constructed sub-grid velocity depends on the stretching parameter d , which is related to the fractal dimension of the signal. In Scotti and Meneveau (1999) [120], it was assumed that d is constant in space and time for homogeneous and isotropic turbulence. Basu et al. (2004) [19] proposed an extension of this work by developing

a multiaffine fractal interpolation scheme where two different values of the stretching parameter was used. They showed that it preserves the higher-order structure functions and the non-Gaussianity of the probability density function (PDF) of velocity increments. They performed extensive analyses of atmospheric boundary layer data and argued that the multiaffine closure model should give satisfactory performance in LES. Marchioli et al. (2008) [80] used fractal interpolation and approximate deconvolution technique to model sub-grid scale turbulence effects on particle dynamics in wall-bounded turbulence. They showed that FIT appears to be inefficient in reintroducing the fluid velocity fluctuation when a constant stretching parameter is assumed [118]. They concluded that an accurate sub-grid model for particles may require information on the higher-order moments of the velocity field [80].

Characteristic features of atmospheric turbulence are the inhomogeneity due to buoyancy and the presence of internal and external intermittency. Intermittency (internal and external) is defined in the first part of this work. For clarity, it is recalled here that internal intermittency means that large velocity gradients are present at small scales and the PDF of velocity differences at high Reynolds number is stretched exponentially at small scales [52]. External intermittency refers to the co-existence of both laminar and turbulent regions in the flow. These attributes make it difficult to synthesize sub-grid velocity field using fractal interpolation since the local stretching parameters have been shown to change randomly in space and time [5, 80].

6.3 Overview

As a new contribution in this part of the thesis, the FIT with random stretching parameters is used to reconstruct inertial-range (sub-grid) scales for LES. The local value of d is computed using Mazel and Hayes [83] algorithm and its PDF is calculated from DNS data of stratocumulus-topped boundary layer, LES data in the same flow configuration and airborne dataset from POST campaign. It was discovered that the PDFs of d collapsed into one curve, independent of the Reynolds number if 1D intersections of velocity fields are low-pass filtered to inertial range wave-numbers. Also, the autocorrelation of d in time is examined. I discover that d decorrelates with the characteristic timescale τ_η and can be chosen randomly after each time step in LES where time steps are considerably larger. The performance of the new approach was compared with FITs with constant values of d through their energy spectra and PDFs of velocity increments. FIT with random values of d performs better than FITs with constant values when applied on the three datasets (DNS, LES and POST). The

issue of mass conservation and the computational requirement of FIT is discussed. To conclude, possible applications of FIT were addressed. *A priori* LES test shows that FIT can reconstruct the resolved stresses L_{ij} of a test filter (which represent the contribution of scales whose length is between the LES grid width and the coarser LES grid width to the Reynold stress) and residual kinetic energy. Also, based on the preliminary test, FIT can improve LES velocity field used in the super-droplet method [125] for the simulation of cloud microphysics.

Part 2 of this thesis is organized as follows. Description of the fractal subgrid-scale model is presented in chapter 7. It starts with a short description of FIT and how the local value of d is computed with Mazel and Hayes [83] algorithm. It continues with a brief description of the POST airborne campaign and LES of stratocumulus topped boundary layer. It shows the comparison between the PDFs of d computed from DNS, LES and POST datasets. It concludes with evaluating the autocorrelation function of d in time. In chapter 8, the new FIT with random values of d is compared with FITs with constant value of d . It shows the application of the new FIT approach to 3D LES velocity fields and addresses the deviation of FIT velocity fields from mass conservation. It ends with an investigation on the computational cost required by FIT. Chapter 9 outlines possible applications for the new FIT model. It explains how the resolved stresses for a test filter and residual kinetic energy can be reproduced with the FIT. It also explores the reconstruction of inertial-range subgrid scales for the Lagrangian tracking of super-droplets in LES velocity field.

Chapter 7

Fractal subgrid scale model - description

In this chapter, a brief description of the fractal interpolation technique (FIT) is presented. It will also describe the improvement to FIT, which can be used to obtain better results in LES of moderate or high Reynolds number turbulent flows. I proceed by accounting for the spatial and temporal variability of the stretching parameter: first, its local value is computed with a method proposed by Mazel and Hayes [83]. Three examples of complex turbulent flows are investigated, first moderate Reynolds number DNS velocity field of stratocumulus-top boundary layer (STBL) [86], second, LES of stratocumulus cloud at Re comparable with atmospheric turbulence [99] and, finally, experimental data from POST airborne measurements in stratocumulus clouds [42, 55, 78]. The PDFs of their local stretching parameter are compared. Second, the autocorrelation of the stretching parameter in time is computed, using DNS dataset of forced isotropic turbulence, downloaded from Johns Hopkins Turbulence Databases (JHTDB) (<http://turbulence.pha.jhu.edu/>).

7.1 Fractal interpolation techniques

The FIT is an iterative affine mapping procedure to construct the synthetic (unknown) small-scale eddies of the velocity field $\mathbf{u}(\mathbf{x}, t)$ from the knowledge of a filtered or coarse-grained field $\tilde{\mathbf{u}}(\mathbf{x}, t)$ [120]. The underlying assumption of the model is the existence of fractal-scale similarity of velocity fields. For clarity, if $\hat{\tilde{\mathbf{u}}}(\mathbf{x}, t)$ have resolution Δ' while $\tilde{\mathbf{u}}(\mathbf{x}, t)$ have Δ such that $\Delta' > \Delta$, the mapping operator $W[.]$ applied to $\hat{\tilde{\mathbf{u}}}(\mathbf{x}, t)$ gives $\tilde{\mathbf{u}}(\mathbf{x}, t) = W[\hat{\tilde{\mathbf{u}}}(\mathbf{x}, t)]$. To generate synthetic small scale velocity fields, the mapping is performed many times i.e. a fractal synthetic field

$$\mathbf{u}_f(\mathbf{x}, t) = \lim_{n \rightarrow \infty} W^{(n)}[\tilde{\mathbf{u}}(\mathbf{x}, t)] \equiv \lim_{n \rightarrow \infty} W[W[W...W[\tilde{\mathbf{u}}(\mathbf{x}, t)]...]].$$

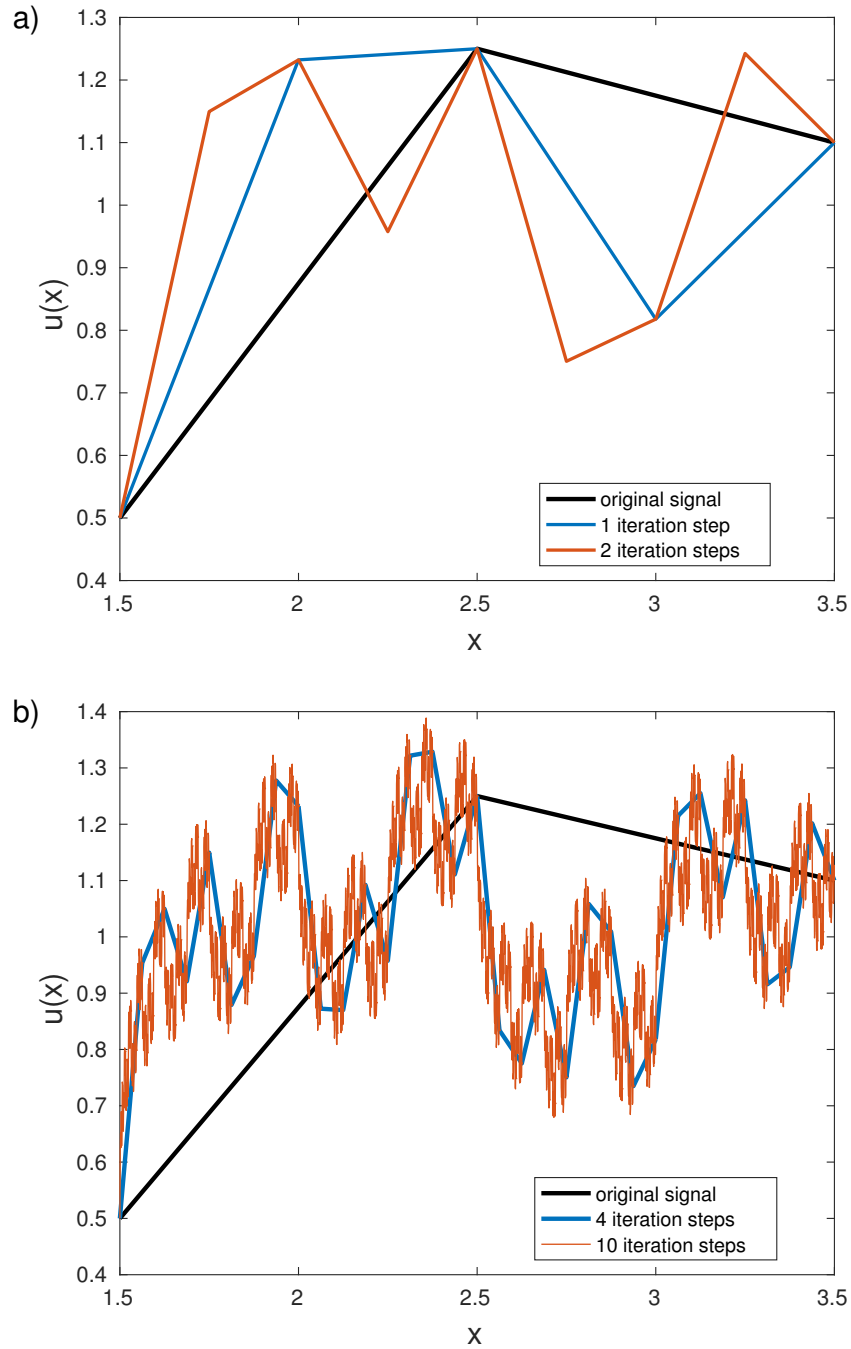


Figure 7.1: Different stages during the construction of a fractal function with stretching parameter $d = \pm 2^{-1/3}$ which interpolates between $(x_i, \bar{u}_i) = (1.5, 3.5)$ to $(x_i, \bar{u}_i) = (0.5, 1.1)$ after (a) 0,1 and 2 reconstruction steps (b) 0, 4 and 10 reconstruction steps.

For example, if three interpolating points $\{(x_i, \tilde{u}_i), i = 0, 1, 2\}$ is considered, the fractal interpolation reconstructs a signal w_j , $j = 1, 2$ at two additional points placed

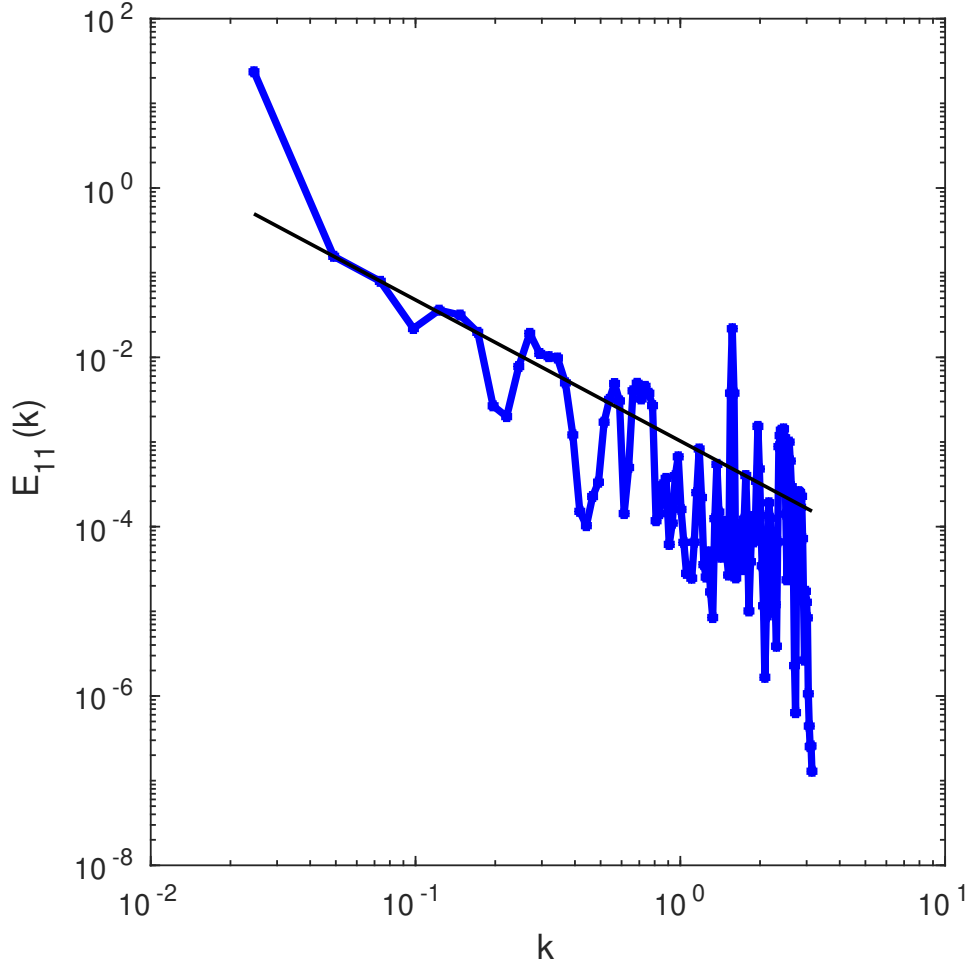


Figure 7.2: Different stages during the construction of a fractal function with stretching parameter $d = \pm 2^{-1/3}$ Energy spectrum of the reconstructed signal after 10 iterations showing $-5/3$ slope.

between points 0 and 1 and points 1 and 2, see figure 7.1. Here, w_j has the following transformation structure:

$$w_j \begin{pmatrix} x \\ u \end{pmatrix} = \begin{bmatrix} a_j & 0 \\ c_j & d_j \end{bmatrix} \begin{pmatrix} x \\ u \end{pmatrix} + \begin{pmatrix} e_j \\ f_j \end{pmatrix}, \quad j = 1, 2 \quad (7.1)$$

with constraints

$$w_j \begin{pmatrix} x_0 \\ \tilde{u}_0 \end{pmatrix} = \begin{pmatrix} x_{j-1} \\ \tilde{u}_{j-1} \end{pmatrix} \quad \text{and} \quad w_j \begin{pmatrix} x_2 \\ \tilde{u}_2 \end{pmatrix} = \begin{pmatrix} x_j \\ \tilde{u}_j \end{pmatrix}, \quad j = 1, 2 \quad (7.2)$$

The parameters a_j, c_j, e_j and f_j can be written in terms of d_j (called the stretching parameter) and the interpolation points $\{(x_i, \tilde{u}_i), i = 0, 1, 2\}$. Values of d_j fix the vertical stretching of the left and right segments at each iteration. It determines the

attribute of the reconstructed signal and is related to the fractal dimension of the signal. Their values are independent of the interpolation points.

The iterative procedure in the limit $n \rightarrow \infty$ creates a continuous function $\mathbf{u}_f(\mathbf{x})$ provided that the stretching parameter d_j obeys $0 \leq |d_j| < 1$. Also, if $|d_1| + |d_2| > 1$ and $(x_i, \tilde{u}_i)$, are not collinear, then the fractal dimension D of the reconstructed signal is the unique real solution of $|d_1|a_1^{D-1} + |d_2|a_2^{D-1} = 1$ (for proof, see [18]). Thus, once the stretching parameter is chosen, the remaining parameters a_j, c_j, e_j and f_j are given as

$$a_j = \frac{x_j - x_{j-1}}{x_2 - x_0} \quad (7.3)$$

$$e_j = \frac{x_2 x_j - x_0 x_j}{x_2 - x_0} \quad (7.4)$$

$$c_j = \frac{\tilde{u}_j - \tilde{u}_{j-1}}{x_2 - x_0} - d_j \frac{\tilde{u}_2 - \tilde{u}_0}{x_2 - x_0} \quad (7.5)$$

$$f_j = \frac{x_2 \tilde{u}_{j-1} - x_0 \tilde{u}_j}{x_2 - x_0} - d_j \frac{x_2 \tilde{u}_0 - x_0 \tilde{u}_2}{x_2 - x_0} \quad (7.6)$$

Given that

$$1 < \sum_{j=1}^N |d_j| < 2, \quad (7.7)$$

where $N + 1 = N_A$ and N_A is the number of anchor points (here, $N = 2$), the stretching parameter d_j relates to the fractal dimension D of a velocity field as:

$$D = 1 + \log_N \sum_{j=1}^N |d_j| \quad (7.8)$$

(for proof, see [17, 18]). It is important to note that the relation between the fractal dimension and the inertial-range self-similarity of turbulent velocity field is not trivial. Orey [97] proved that almost all realizations of a Gaussian random field with a power-law spectrum, $E(k) \sim k^{-\alpha}$ with $1 < \alpha < 3$, give fractal dimension $D = (5 - \alpha)/2$. For Kolmogorov spectrum, $\alpha = 5/3$, which results in $D = 1.67$. Although turbulent velocity fluctuations are not Gaussian, the high-Reynolds experimental results of Praskovsky et al. [110] and Scotti et al. [121] agree with Orey's theorem. They concluded that turbulent velocity fluctuations gives a fractal dimension $D \simeq 1.7 \pm 0.05$, which is close to $D = 1.67$ expected for Gaussian signals.

If a fractal dimension of $5/3$ relating to $-5/3$ Kolmogorov scaling in the inertial-range of velocity fields is assumed, then $d_j = \pm 2^{-1/3}$ (if d_j is assumed to be the

same for all grid spacings) [120]. Figure 7.1a-b shows the 1-D construction of w_j . It starts with a signal containing three grid points and successively apply the map w_j with stretching parameter $d_j = \pm 2^{-1/3}$. Shown are the initial signal, first, second, fourth and the tenth application of the map w_j . The energy spectrum after ten reconstruction steps is shown in figure 7.2.

In 3-D, FIT is performed separately along x -, y - and z - directions, see [120]. Assuming that the filtered field has N grid points in all three directions i.e. $\tilde{\mathbf{u}}_{ijk}$ for $i, j, k = 0, 1, 2, \dots, N - 1$. First, 1-D intersections of the coarse-grained field $\tilde{\mathbf{u}}_{ijk}$ along x - direction are created and FIT is performed for each 1-D intersection (see the blue lines on the schematic figure 7.3), that is, for each $j, k = 0, 1, \dots, N - 1$. A field, denoted as $\tilde{\mathbf{u}}_{ijk}^x$, where $i = 0, 1, \dots, 2N - 1, j, k = 0, 1, \dots, N - 1$, is obtained. Then, FIT for each 1-D intersection of $\tilde{\mathbf{u}}_{ijk}^x$ along y - direction is performed, which gives a field $\tilde{\mathbf{u}}_{ijk}^{x,y}$, where $i, j = 0, 1, \dots, 2N - 1, k = 0, 1, \dots, N - 1$ (red lines in figure 7.3). Lastly, FIT is performed on $\tilde{\mathbf{u}}_{ijk}^{x,y}$ along z - direction similar to how it was performed in x - and y - directions. With this, the field $\mathbf{u}_{ijk}$, where $i, j, k = 0, 1, \dots, 2N - 1$ is finally obtained.

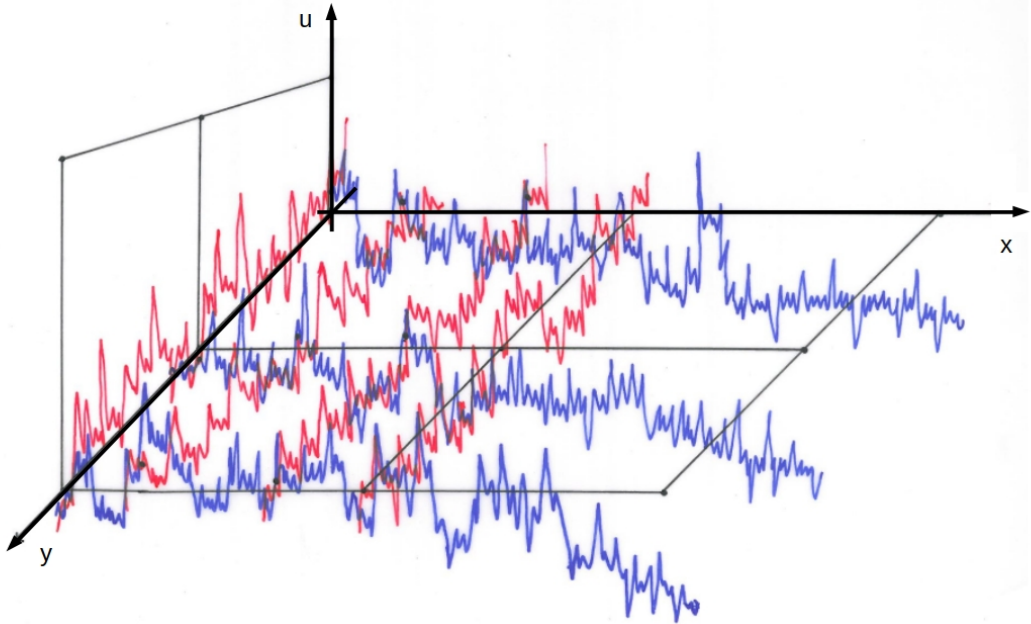


Figure 7.3: Schematic picture of a process of the fractal reconstruction in 2D. Courtesy to Z. Waławczyk

7.2 Stretching parameter estimation

Mazel and Hayes (1992) [83] proposed an algorithm for computing the local stretching parameter d_i of any given arbitrary dataset. The algorithm is based on the property that the resulting fractal field is self-similar. For illustration, if we consider a dataset with 5 interpolation points $\{(x_i, u_i), i = 0, 1, 2, 3, 4\}$, let μ be the vertical distance between the middle interpolation point (x_2, u_2) and a straight line between the end points (x_0, u_0) and (x_4, u_4) , see figure 7.4. The value of μ is positive if the interpolation points are above the straight line and negative otherwise. Let ν_1 be the vertical distance between (x_1, u_1) and a straight line between (x_0, u_0) and (x_2, u_2) while ν_2 be the vertical distance between (x_3, u_3) and a straight line between (x_2, u_2) and (x_4, u_4) . Both ν_1 and ν_2 are positive if their respective interpolation points are above their respective straight lines and negative otherwise. Then the stretching parameters d_1 and d_2 are ν_1/μ and ν_2/μ , respectively. An illustration of this calculation is presented in figure 7.4.

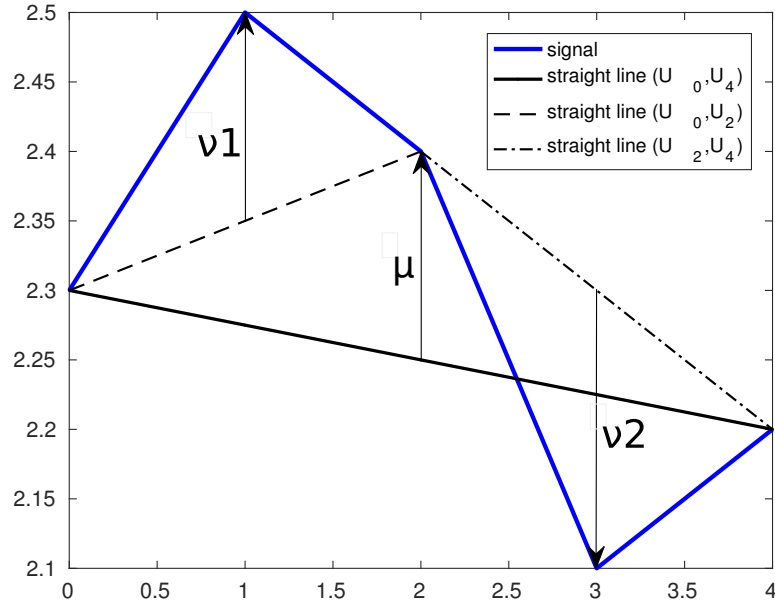


Figure 7.4: Illustration of the stretching parameter calculation.

To see how the local values of d vary in space (or time), this algorithm is applied on a 1-D intersections of DNS velocity field of STBL (see section 4.2.1 for details of this simulation) [5, 6]. Figure 7.5a shows the local values of d . There is a significant variation of d , with some values outside the interval $(-1, 1)$, due to the intermittent

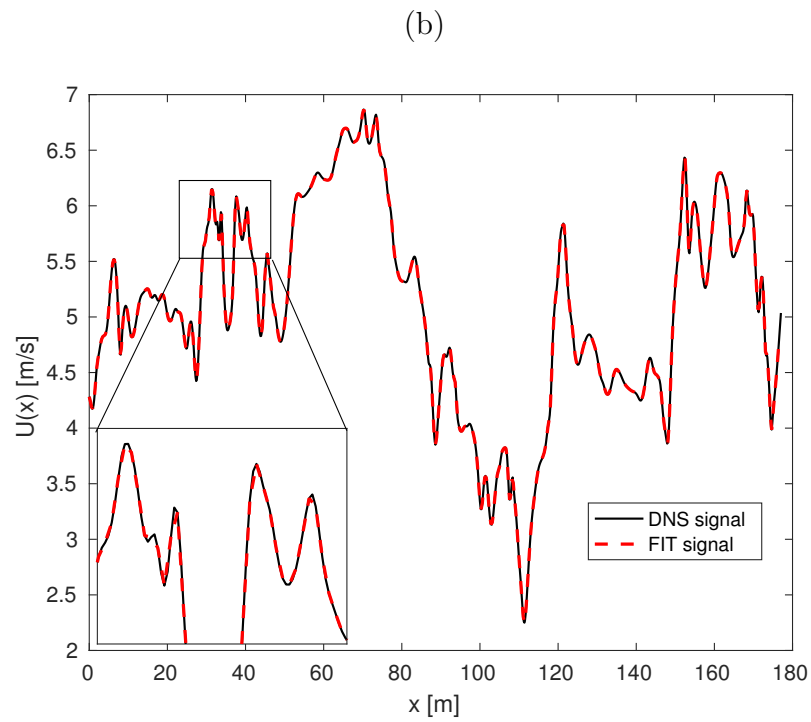
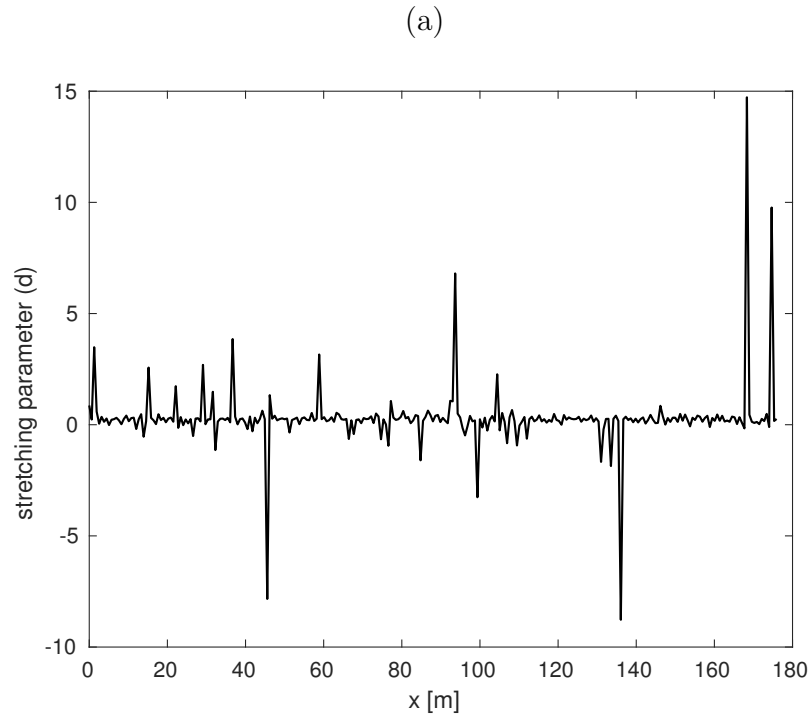


Figure 7.5: a) Variability of local stretching parameters d in 1D DNS velocity signals
b) 1D DNS velocity signals showing the original and the FIT reconstructed signal using local values of d in (a)

nature of turbulent velocity fields. To verify the applied procedure, the resolution of the signal is reduced from Δ to 2Δ and FIT is applied (as described in section 7.1) once with local values of d as given in figure 7.5a. As expected, the FIT constructed signal is identical with the original one, see figure 7.5b.

As described in Section 7.1, to assure continuity of the reconstructed signal in the limit of $n \rightarrow \infty$ reconstruction steps, d should take values within the interval $(-1, 1)$. In order to satisfy this condition, the constraint $|d| \leq 1$ is set in the calculation of local stretching parameters, i.e. d values outside this interval are neglected.

Applying d as a variable stretching parameter to FIT changes slightly the properties of the FIT. These properties (such as smoothness, sensitivity to perturbation and stability) were studied by Wang and Yu (2013) [146]. They concluded that FIT with variable parameter d displays less self-similarity, is more flexible, stabler to small perturbation and more suitable for the approximation of many non-stationary experimental data than the use of constant d [123, 146]. Although Wang and Yu (2013) provide a theoretical basis for FIT with variable stretching parameter, to the best of the author’s knowledge, such approach was not applied before to turbulent flows.

7.3 Description of airborne and LES datasets

This section provides a brief description of POST airborne campaign and LES of stratocumulus cloud top. The DNS of stratocumulus boundary layer was described in section 4.2.1.

7.3.1 POST airborne data

In the following analysis, physics of stratocumulus-top (POST) airborne data is used. The focus is on high-resolution in situ measurements of wind velocity fluctuations (time signals) from one of the flight segments in the stratocumulus top boundary layer. This segment was a part of flight 13 of the POST research campaign [42, 78] carried out in the vicinity of Monterey Bay in July and August 2008 (the data are available online via <https://www.eol.ucar.edu/projects/post/>). The signal’s sampling frequency was 40 Hz (corresponding to ~ 1.4 m spatial resolution) and the duration was $T = 438.75$ s. The magnitude of the vector difference between the wind and aircraft velocity, averaged over the track vector, was 55 ms^{-1} and the turbulence intensity $u' = 0.28 \text{ ms}^{-1}$. Turbulence kinetic energy dissipation rate was estimated from the power spectral density and the second-order structure function in Ref. [55]. For flight 13, the average value in the well-mixed cloud top layer was $\epsilon =$

$0.55 \cdot 10^{-3} \text{m}^2/\text{s}^3$. The kinematic viscosity at the flight height was $\nu = 1.46 \cdot 10^{-5} \text{m}^2/\text{s}$. With this, the Taylor microscale equals, approximately $\lambda \approx 0.19 \text{ m}$ and $Re_\lambda \approx 3900$ is around 20 times larger than in the DNS described in Section 4.2.1.

7.3.2 LES of stratocumulus-top boundary layer

The large eddy simulation of stratocumulus top boundary layer for POST flight 13 in Ref. [99] was performed with a simplified version of 3-D non-hydrostatic anelastic Eulerian-semi-Lagrangian (EULAG) model [112] without sub-grid scale (SGS) model (also called implicit LES). In implicit LES, the truncation terms of the numerical scheme account for the effect of unresolved turbulence. In previous works [54, 100, 135] it was shown that implicit LES performs comparable to conventional LES (with SGS model). The code solves the three velocity components ($\mathbf{u} = (u, v, w)$) in x -, y - and z - directions with other atmospheric variables such as potential temperature θ etc (in equations 2.25 to 2.29). The velocity components were advected using the Multidimensional Positive Definite Advection Transport Algorithm (MPDATA) [128].

The computational domain is 3 km in x and y directions and 1.2 km in z direction with a grid resolution of 5 m in each directions. The flow is periodic across the horizontal boundaries and impermeable free slip condition is applied at the upper boundary. The lower boundary is impermeable with partial slip conditions imposed through near-surface momentum fluxes. The initial values of u and v velocity components were set to the geostrophic wind $U_g = 5.0 \text{ m s}^{-1}$ and $V_g = -7.0 \text{ m s}^{-1}$, respectively with small disturbances. The time step δt was chosen such that the maximum value of the Courant number throughout the simulation period and computational domain is ~ 0.5 . For details, readers are referred to Ref. [99]. Figure 7.6 shows u velocity component along the horizontal and vertical cross-sections of the flow field. The cloud top region is placed at the vertical height $z \sim 700 \text{ m}$. Above this region is the free troposphere, which is warm and unsaturated with low turbulence intensity while the region below the cloud top is moist, saturated with high turbulence intensity. Vertical profile of mean velocity field and r.m.s. of horizontal and vertical velocity fluctuations are shown in figure 7.7.

7.4 Probability distribution function of the stretching parameter

In this section, velocity field dataset from numerical simulations and experiment described in Section 7.3 will be analyzed. Stretching parameters are extracted, as

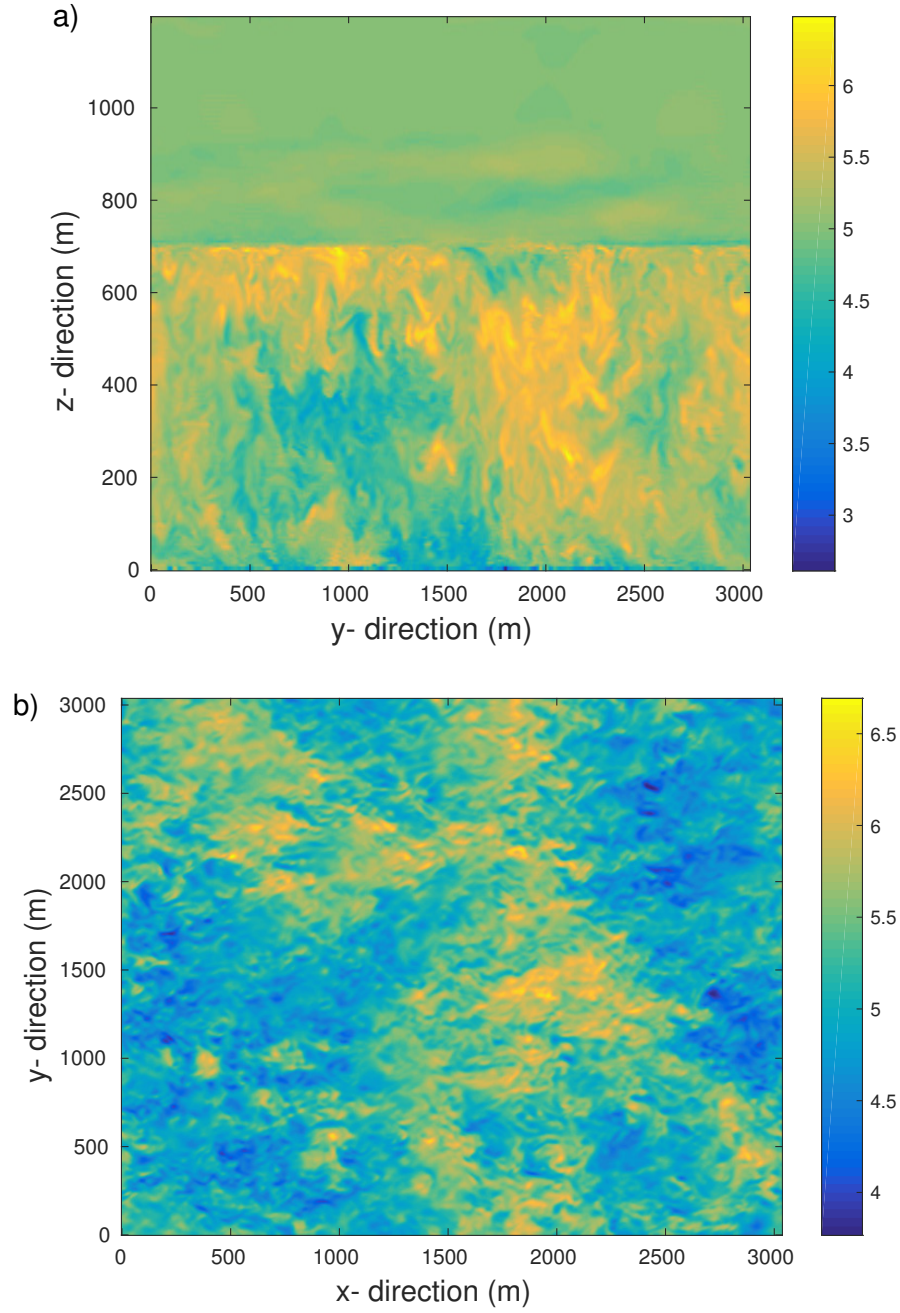


Figure 7.6: Velocity component u of LES field. (a) Vertical cross section at $y = 1595$ m. (b) Horizontal cross section at $z = 595$ m

discussed in Section 7.2 and the PDFs of the module of $|d|$, denoted as $f(|d|)$ are calculated. Here, d stands for the sample space variable of the stretching parameter d .

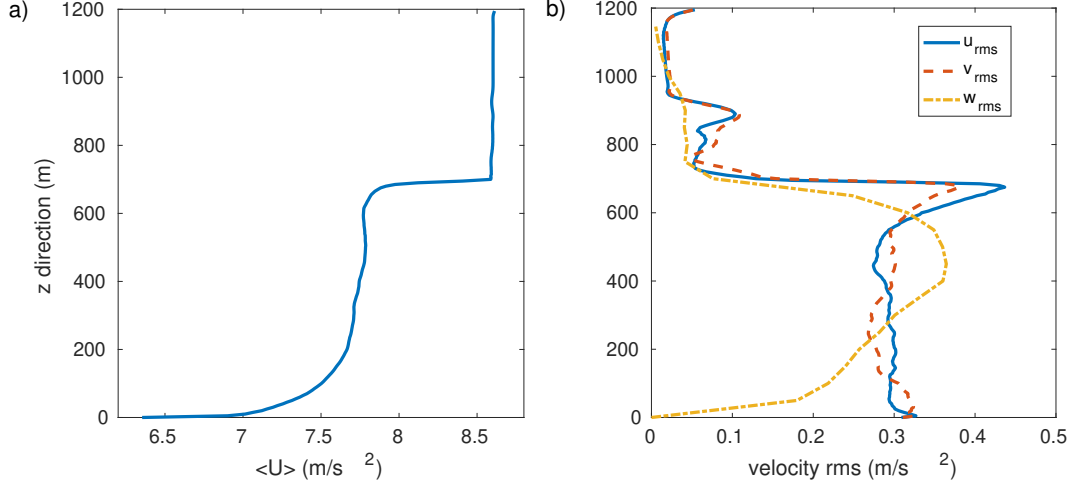


Figure 7.7: Statistics of LES velocity field (a) vertical profile of mean velocity (b) vertical profile of velocity root-mean-square

7.4.1 DNS of stratocumulus-top mixing layer

For DNS data described in Section 4.2.1, I use horizontal profiles of the u , v and w components of velocity at a height corresponding to the in-cloud region ($z = 550m$). First, the variability of d is investigated as 1-D intersections of DNS velocity field are filtered successively to wavenumber in the inertial range. Starting with the fully resolved DNS field with the grid spacing equal to η_0 , the resolution is reduced to $2\eta_0$ using a low-pass filter and the local values of d are calculated for the filtered velocity field. Then, the velocity signal is filtered to a grid resolution of $4\eta_0$ etc., the cut-off wavenumber is decreased, until the resolution matches the inertial-range (at about $16\eta_0$ to $128\eta_0$). After each filtering, the local values of d are extracted. The low-pass filter used is the finite impulse response (FIR) filter of order 30 designed using the Hamming window method [149]. This is done with decimate function in MATLAB[®] software. The reasons for the use of the decimation low-pass filter are to effectively downsample the signal (i.e reduce the number of grid points) and guard against aliasing. The downsampling feature of the filter was important to have a reconstructed signal with the same number of grid points as the original (DNS, LES or POST airborne) signal. The local estimate of d is calculated with the algorithm explained in section 7.2. Stretching parameter values outside the interval $(-1, 1)$ are neglected and absolute value of d is used to calculate its PDF. Since the flow is statistically homogeneous over horizontal planes, similar results are obtained for 1D intersections of velocity field calculated either in x - or y - directions.

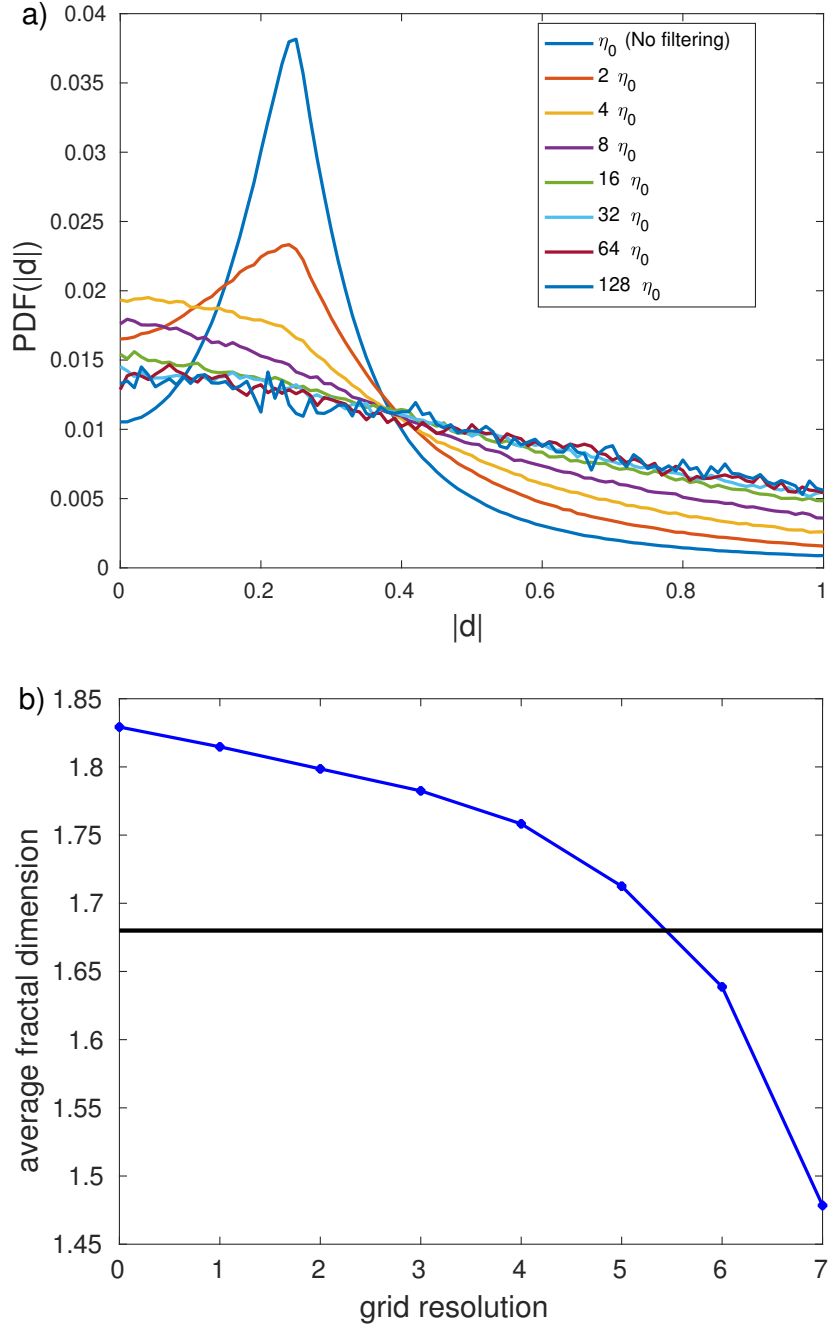


Figure 7.8: (a) PDFs of the absolute value of stretching parameter for horizontal profile of DNS velocity at different resolutions. (b) The average fractal dimension for horizontal profile of DNS velocity at different resolutions. The black line shows the value corresponding to the $-5/3$ inertial-range scaling.

Figure 7.8 presents the PDF of $|d|$ and average fractal dimension (from equation (7.8)) of DNS velocity signals at different grid resolutions. In figure 7.8a, the PDFs

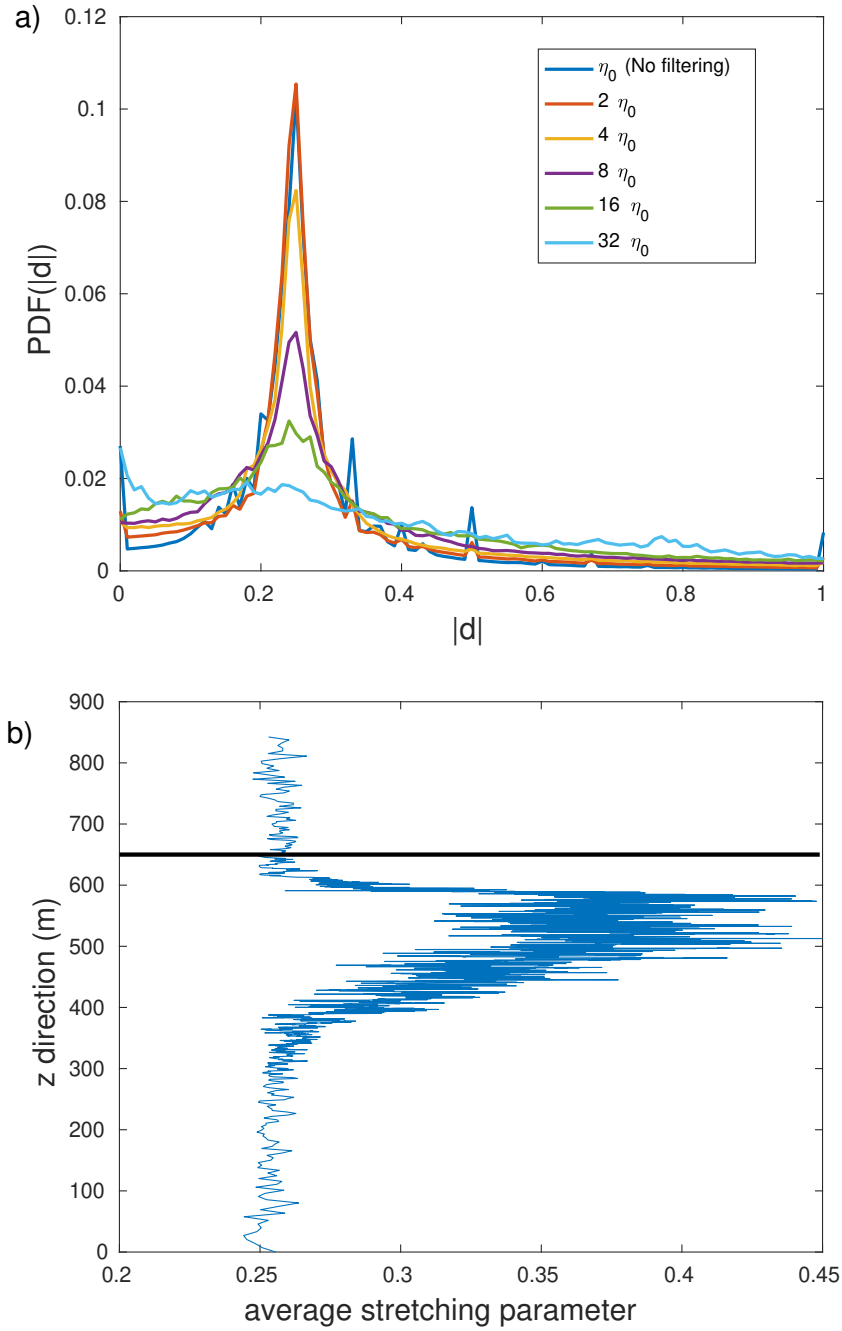


Figure 7.9: (a) PDFs of the absolute value of stretching parameter for vertical profile of DNS velocity at different resolutions. Inertial-range wavenumbers correspond to iteration 4 and 5 (b) The average stretching parameter for vertical profile of DNS velocity. The black line indicates approximately the cloud-top region.

change significantly for the first four successive filtering steps but seem to be self-similar when filtered successively to inertial-range wavenumbers (at steps 4 to 7).

All the three velocity components give similar profiles of the PDF of the stretching parameter. The average fractal dimension, calculated according to Eq. (7.8), decreases to $-5/3$ inertial range scaling, as seen in figure 7.8b. The calculated vertical profile of averaged $|d|$ across the STBL (see figure 7.9b) is smaller than 0.6 or 0.7 reported in Ref. [118] even in the core cloud region (at $z \approx 550$ m). This result is expected due to the presence of external intermittency (laminar regions will give zero or close to zero local values of d). Even in the in-cloud region the volume fraction occupied by turbulent flow is smaller than one and equals approximately $\gamma = 0.9 - 0.95$, where γ is the intermittency parameter, see section 5.2.3 [8]. Due to small values of γ in the outer-cloud regions, the average value of d also decreases therein to, approximately 0.25, see figure 7.9b.

In Ref. [120], it was shown that a fractal signal will only dissipate energy in the limit of small viscosity if $|d| > 0.5$. So as to retain dissipative properties, $|d| < 0.5$ are neglected in further sub-grid scale reconstruction in section 8.1. If only $|d| > 0.5$ is considered, the average stretching parameter will be similar to values obtained in Ref. [118].

No self-similarity of PDFs of $|d|$ is observed in the vertical z - direction, see figure 7.9a. Here, velocity field was filtered to a grid resolution of $16\eta_0$ or $32\eta_0$. This is due to the anisotropy of turbulence caused by large scale shear production and buoyancy. Similar conclusion was made by Marchioli et al. [79, 80] where the locally computed stretching parameters varied significantly in the wall-normal direction. Also, in that study, the average stretching parameter was lower than that obtained experimentally from homogeneous isotropic turbulence.

There is no significant variation in the horizontally calculated average of d in the in-cloud region - at $450m \leq z \leq 550m$ (see figure 7.9b). Hence, the remaining analysis is based on the horizontal profiles in this region, where turbulence is close to isotropic. Also, the probabilities of having positive or negative stretching parameter are equal.

7.4.2 Comparison with LES and POST data

To investigate the variability of the stretching parameter in high Reynolds number turbulence, d are computed from LES field and the POST airborne dataset using the Mazel and Hayes' algorithm described in section 7.2. The PDF of $|d|$ from LES and POST data will be compared with the respective profile from the DNS. DNS velocity field is filtered with the decimate function [149] (described in section 7.4.1) to a spatial resolution of $16\eta_0$ (equivalent to 1.6 m). For LES, the horizontal profile of u velocity

component at $z = 595\text{m}$ (corresponding to the in-cloud region with the maximum turbulent intensity) is used to estimate stretching parameters. Numerical scheme of LES introduces a spurious damping of the energy of the smallest resolved scales [157]. In order to remove these effects, I filtered the LES velocity field with the decimate function (described in section 7.4.1), to a grid resolution of 20 m (corresponds to inertial-range wavenumber) from its 5 m grid resolution. Another possibility, instead of filtering, would be to recover the energy of the smallest scales using the approximate deconvolution method - ADM (see [157] for details). Combining the ADM and the FIT is, however, left for further work and will not be addressed here. The POST airborne data is filtered from its frequency of 40 Hz to 10 Hz (corresponding to a spatial resolution of 5.6 m) so as to eliminate measurement errors. The sampling frequency of 10 Hz is already within the inertial-range. All the three u , v and w components of POST velocity dataset are combined to form a large dataset since their individual PDF of $|d|$ are similar.

As seen in Fig. 7.10 comparison between LES and DNS profiles is very good, in spite of different Reynolds numbers of the two simulations. The PDF of $|d|$ from POST data seems to oscillate around the respective DNS profile. Some differences observed may be due to the effect of large scale tendencies on measured airborne data and small scale measurement noise. Based on the results shown in Fig. 7.10, it can be concluded that the PDF of the stretching parameter in the inertial range is a universal function, independent of the Reynolds number, at least, if turbulence is close to isotropic (in the core-region of the cloud).

7.5 Autocorrelation of the stretching parameter in time

For proper application of the fractal sub-grid model in LES of turbulent flows, it is crucial to know how the stretching parameter d decorrelates in time. This leads to the calculation of the autocorrelation function of $d(\mathbf{x}, t)$

$$R^d(\tau) = \langle d(\mathbf{x}, t_0)d(\mathbf{x}, t_0 + \tau) \rangle_x$$

where $\tau > 0$ is the time increment between the two times t_0 and $t_0 + \tau$ and $\langle \dots \rangle_x$ is the spatial average defined in equation 2.19. For this analysis, the DNS of forced isotropic turbulence is used. The data are obtained on a 1024^3 periodic grid, using a pseudo-spectral parallel code. The velocity field is downloaded from Johns Hopkins

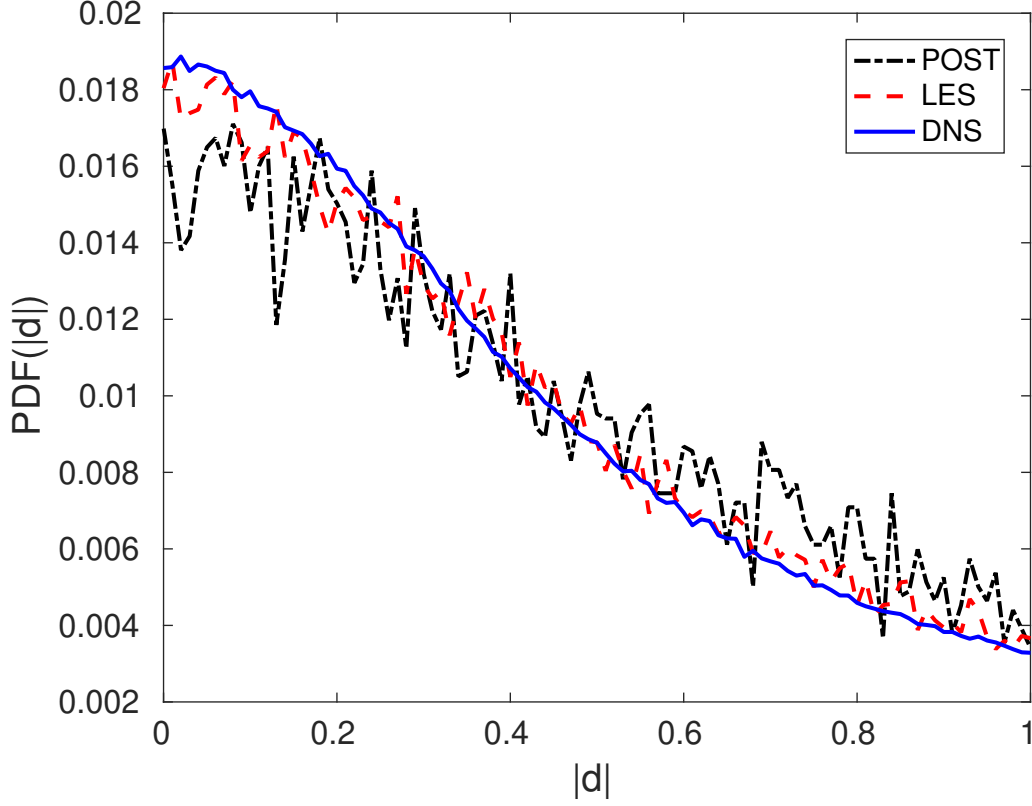


Figure 7.10: Probability distribution of the absolute value of the stretching parameter $|d|$ from filtered DNS, LES velocity signals of stratocumulus cloud-top and POST data. DNS and LES velocity fields are filtered with wavenumber within the inertial range.

Turbulence Databases (JHTDB) (<http://turbulence.pha.jhu.edu/>). The Taylor-scale Reynolds number R_λ of the flow is 418. The simulation has an integral scale $L = 1.36$, dissipation rate $\epsilon = 0.103$, rms velocity $u' = 0.686$, Kolmogorov length scale $\eta = 0.0028$ and Kolmogorov time scale $\tau_\eta = 0.04$. The DNS spatial and time resolution is $2\pi/1024$ and 0.002 respectively. A total of 5024 time samples of the velocity field are used.

First, velocity fields for all time instants was filtered to grid resolution of 16η (corresponding to the inertial-range scales). Then, $d(\mathbf{x}, t)$ and its autocorrelation is calculated from the velocity fields using Mazel and Hayes' algorithm explained in section 7.2. Figure 7.11 shows the autocorrelation function $R^d(\tau)$ of d and the autocorrelation function $R^{\delta\mathbf{u}}(\tau)$ of the velocity increment $\delta\mathbf{u}$ defined as $\delta\mathbf{u} = \mathbf{u}(\mathbf{x} + \mathbf{r}, t) - \mathbf{u}(\mathbf{x}, t)$. The autocorrelation of $\delta\mathbf{u}$ is calculated in a similar way as the one of $d(\mathbf{x}, t)$. It is observed that the stretching parameter decorrelates with the characteristic time scale

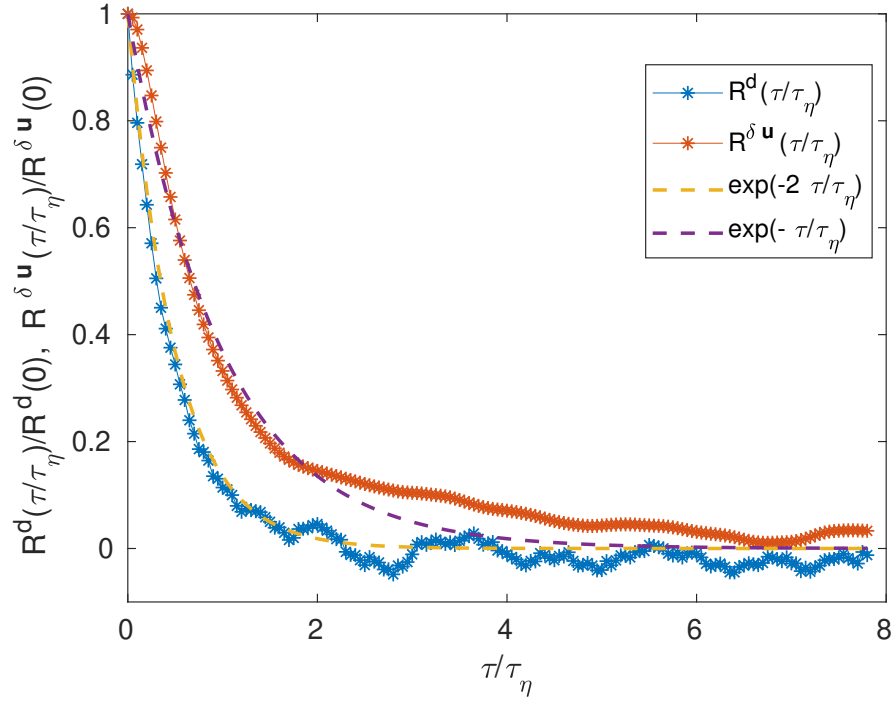


Figure 7.11: Autocorrelation function $R^d(\tau/\tau_\eta)$ for the stretching parameter and autocorrelation function $R^{\delta\mathbf{u}}(\tau/\tau_\eta)$ for the velocity increment $\delta\mathbf{u}$.

of the order of τ_η , same as that of $\delta\mathbf{u}$. As time steps used in LES are much larger than the Kolmogorov time scales, this implies that the stretching parameter can be chosen randomly after each consecutive time step in LES.

Chapter 8

Fractal subgrid scale model - analysis and validation

In this chapter, the performance of the new FIT approach (explained in chapter 7) is compared with FIT of the constant stretching parameter values from Ref. [120] and the multiaffine fractal interpolation scheme [19]. The PDF of local stretching parameter is used to construct subgrid velocity, starting with the filtered DNS or LES.

The extracted PDF of d is used to perform 3D reconstruction of subgrid eddies. The energy spectra of the reconstructed velocity field and the statistics of velocity increments are calculated. The focus on the statistics of velocity increments is motivated by their ability to quantify internal intermittency of small scale turbulence [52, 59, 70], which can influence inertial particle statistics in turbulent flows [16, 47, 59]. The new approach with random d is the most favourable in terms of the investigated statistics. It reproduces the Kolmogorov's $-5/3$ scaling of turbulent kinetic energy spectra in the inertial range with the smallest error and without spurious modulations. Moreover, similarly as for the multiaffine scheme [19], the reconstructed PDFs of velocity increments have non-Gaussian, stretched tails.

Finally, this model is applied to 3-D LES of stratocumulus-top boundary layer (STBL) [54, 82, 99]. The mass conservation of the FIT reconstructed fields is investigated. Each FIT reconstruction step increases the error in mass conservation, however, this error is still of the same order of magnitude as the error of the filtered LES without FIT. The computational cost of the FIT procedure applied to three velocity components in 3D space is investigated. It is shown that the proposed fractal model is computationally efficient.

8.1 Fractal interpolation of filtered DNS

First, 1D horizontal intersections of DNS velocity field at $z = 550$ m are filtered to a spatial resolution of $16\eta_0 \approx 1.6m$ (which is within the inertial range) using the decimation function described in Section 7.4.1. Sub-filter scales are reconstructed to the resolution η_0 using FIT. For this, the stretching parameter is selected from its PDF calculated from the DNS data, see Fig. 7.10, using the inverse transform sampling method [33]. The procedure is briefly indicated as follows

1. Calculate cumulative distribution function $F(|d|)$ from the PDF $f(|d|)$, as

$$F(|d|) = \int_0^{|d|} f(s)ds.$$

2. Calculate the inverse function $F^{-1}(y)$.
3. If y is a random number from uniform distribution $[0,1]$ then $d = F^{-1}(y)$ is a random number from the investigated PDF.

Apart from the mathematical constraint $|d| \leq 1$, which assures the continuity of the reconstructed signal at $n \rightarrow \infty$ reconstruction steps [18], the second constraint, discussed in Section 7.4.1 was related to the dissipative properties of the signal [121] and reads $|d| > 0.5$. Hence, in practice, in the reconstruction process, only the values $|d|$ that were larger than 0.5 are retained. If $|d| \leq 0.5$ is selected, the procedure is repeated and another random value is chosen, till the condition $0.5 < |d| \leq 1$ is satisfied. Next, the sign of d is selected randomly, such that the positive and negative d have equal probabilities. Under such assumptions, the ensemble average $\langle |d| \rangle$ is comparable to values reported in Ref. [118] and the scaling of the reconstructed energy spectra is close to the theoretical $k^{-5/3}$. Using only one constraint, $|d| \leq 1$, led to underprediction of the reconstructed spectra. Hence, the choice $0.5 < |d| \leq 1$ seems the most favourable as it is supported by the theoretical constraints [17, 121] and gives satisfactory results.

The inertial-range scale invariance is the property that directly relates to the idea of fractality of velocity field. As seen in Fig. 7.8a, profiles of PDF $f(|d|)$ collapse into one curve only for cut-off wavenumbers from the inertial range. For this reason, the fractal reconstruction of the dissipative part of the spectrum is not justified, as no self-similarity is observed there. Instead, in the FIT reconstruction process, the inertial range was extended down to η_0 and properties of such an artificial velocity field are investigated. The lack of the dissipative range could be a possible drawback

if Lagrangian particles are tracked in the reconstructed field. This would concern especially the motion of small-inertia particles which are correlated with smaller eddies [106]. However, in practice, FIT in numerical simulations of high- Re atmospheric flows will be restricted to a few reconstruction steps, due to increased computational time. With this, reconstruction of the signal down to η_0 will not be possible and the smallest resolved scales will belong to the inertial range.

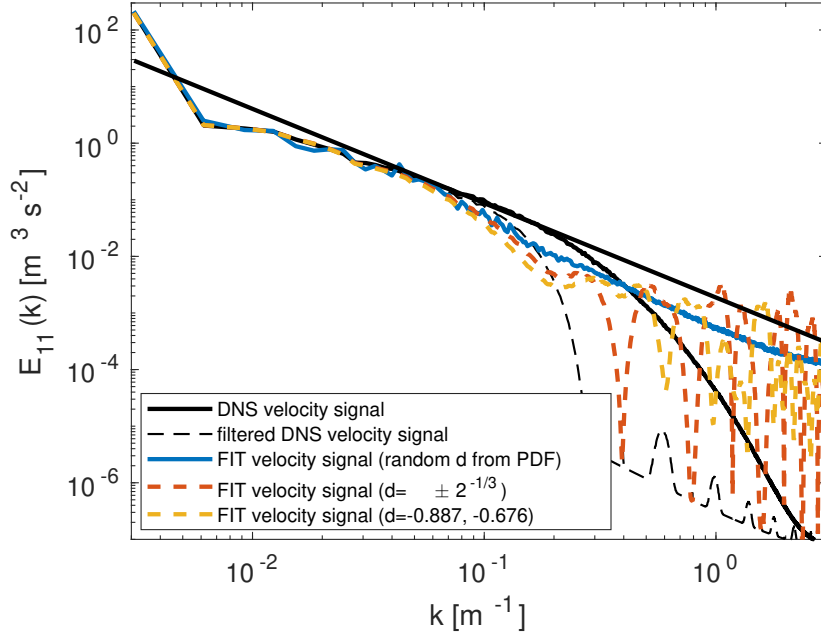


Figure 8.1: Longitudinal energy spectra of u velocity component for DNS and FIT with constant stretching parameter $d = \pm 2^{-1/3}$, with constant stretching parameters $d = -0.887$ and $d = -0.676$ and with random stretching parameters from calculated PDF

Figure 8.1 shows the longitudinal energy spectra $E_{11}(k)$ (for u velocity component along x direction) of DNS, filtered and FIT-reconstructed velocity field for the three investigated versions of the model: with $d = \pm 2^{-1/3}$ as originally proposed by Scotti & Meneveau [120], with $d_1 = -0.887$, $d_2 = -0.676$ as proposed by Basu et al. [19], and with the new proposal with random d . As it is observed, in case of constant values of d energy spectra exhibit periodic modulations (see also figures 7 and 8 of [120]). Basu et al. [19] avoid these modulations by applying the discrete Haar wavelet transform. FIT energy spectrum with constant values of $d = \pm 2^{-1/3}$ is much lower in some wave-numbers than the $-5/3$ inertial-range scaling (especially at wavenumbers close to the cut-off scale), although the upper envelope qualitatively follows the $-5/3$ inertial-range scaling. The FIT energy spectrum reconstructed with constant values of

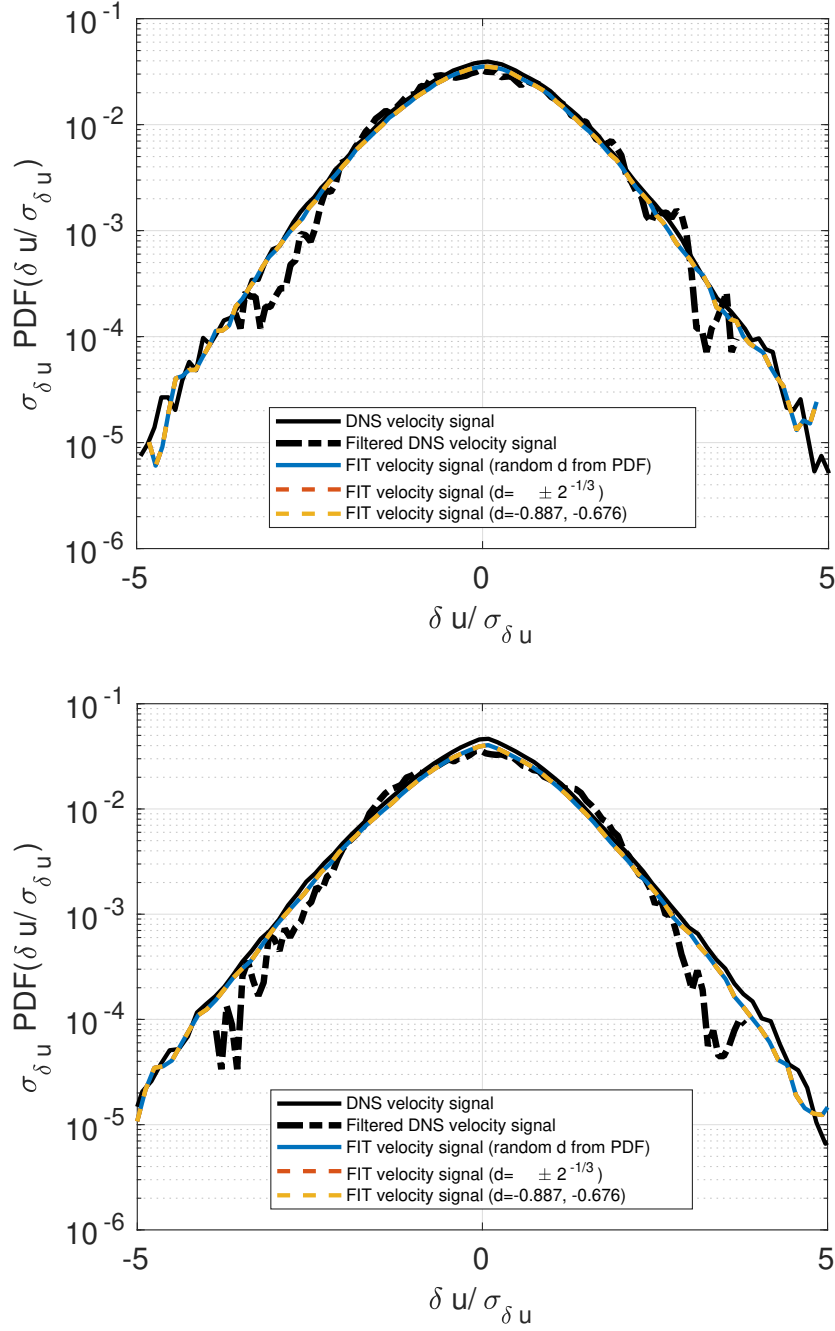


Figure 8.2: PDFs of velocity increments of DNS, filtered DNS and FIT fields at (a) $r = 128\eta_0$, (b) $r = 64\eta_0$ showing the Gaussianity of PDFs at large scales.

$d = -0.887, -0.676$ has similar properties as the Scotti & Meneveau approach, except that the range between the upper and lower envelope of the spectrum is somewhat smaller. The FIT energy spectrum reconstructed with random values of d follows the inertial-range scaling closer and shows no periodic modulations.

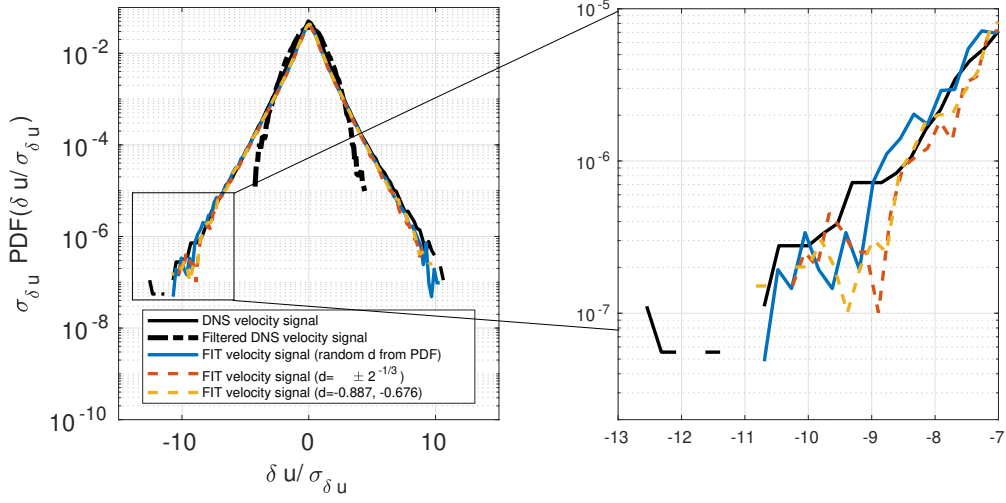


Figure 8.3: PDFs of velocity increments of DNS, filtered DNS and FIT fields at $|\mathbf{r}| = 8\eta_0$ with constant stretching parameter $d = \pm 2^{-1/3}$, $d = -0.887$ and $d = -0.676$ and random stretching parameters from its PDF.

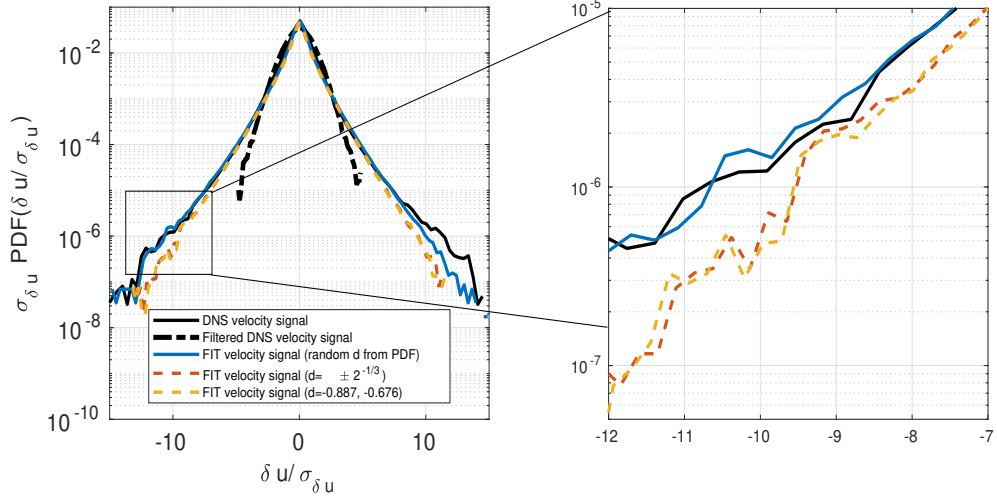


Figure 8.4: PDFs of velocity increments of DNS, filtered DNS and FIT fields at $|\mathbf{r}| = 4\eta_0$ with constant stretching parameter $d = \pm 2^{-1/3}$, $d = -0.887$ and $d = -0.676$ and random stretching parameters from its PDF.

Next, the statistics of velocity increments at two different points $\mathbf{u}(\mathbf{x}+\mathbf{r}, t) - \mathbf{u}(\mathbf{x}, t)$ are investigated. The sample space of velocity increment will be denoted by $\delta\mathbf{u}$, its module by $\delta u = |\delta\mathbf{u}|$ and the distance between points by $r = |\mathbf{r}|$. The tails of the PDFs of velocity increments in the isotropic turbulence $f(|\delta\mathbf{u}|, r, t)$, can be approximated by

$$f(|\delta\mathbf{u}|, r, t) \sim \exp(-A|\delta\mathbf{u}|^c), \quad (8.1)$$

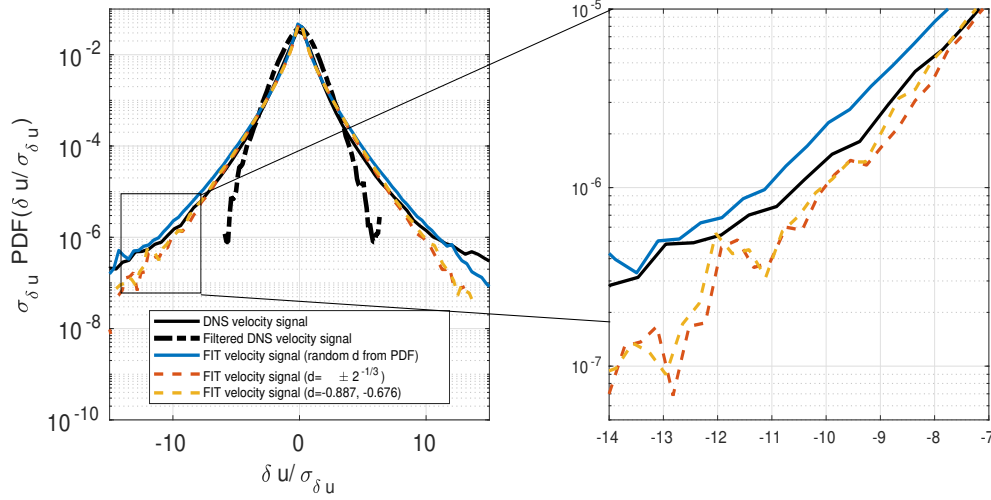


Figure 8.5: PDFs of velocity increments of DNS, filtered DNS and FIT fields at $|\mathbf{r}| = 2\eta_0$ with constant stretching parameter $d = \pm 2^{-1/3}$, $d = -0.887$ and $d = -0.676$ and random stretching parameters from its PDF

where A is a constant and the stretching exponent c varies monotonically from 0.5 for r in the dissipation range to 2 (which is a Gaussian distribution) for r in the integral scale range, see Ref. [58]. The non-Gaussianity of the PDFs for small r indicates the presence of the internal intermittency, that is, the probability of extreme events (large velocity differences) at these scales is much higher than predicted by a Gaussian distribution.

Figure 8.2 presents the PDFs of velocity increment (δu) for DNS, filtered DNS and FIT velocity signals with constant and random values of d for $r = 128\eta_0$ and $r = 64\eta_0$. To increase the size of dataset used to calculate PDFs, both longitudinal (x) and transverse (y) 1D intersections of the velocity field at $z = 550$ m were considered and, additionally, results were averaged over all three velocity components.

All three FIT approaches presented in Fig. 8.2 compare well with the corresponding DNS profiles. PDFs at $r = 128\eta_0$ are clearly Gaussian, see Ref. [52, 70]. Differences are observed when the distance r decreases to $r = 8\eta_0$, $4\eta_0$ and $2\eta_0$, see Figs. 8.3, 8.4 and 8.5, respectively. The PDFs of velocity increments are far from Gaussian and slightly skewed. The FIT model with random d provides the best FIT with the DNS at smaller r .

I note here that $r = 4\eta_0$ and $2\eta_0$ correspond to dissipative-range scales. The intermittency at short r seems to be correctly reproduced, especially by the approach with random d . Although in the reconstruction process, the dissipative range is not reproduced in any of FIT models. The reason for this result could be due to the range

of d values used for the reconstruction. Regions of the flow, in which the values of $|d|$ were greater than 1 or less than 0.5, were replaced with $0.5 < |d| < 1$. This range of d might give velocities of similar magnitude as the DNS at those grid points (even when their values of d were outside this range), leading to the similarity in the PDF of velocity increments at smaller r .

8.2 Fractal interpolation of POST airborne data

In order to test the performance of the sub-grid model on high Reynolds number airborne data, u component of velocity field from flight 13 in POST airborne research campaign [42, 78] is used. The velocity signal is filtered with the decimation function (described in section 7.4.1) from its frequency of $40Hz$ to $10Hz$ (corresponding to the spatial resolution of 5.6 m). The filtering was done to eliminate measurements errors at large frequencies. This filtered signal is used as the reference velocity field to validate the performance of the FIT model. This set has a larger inertial range compared to DNS data analyzed earlier (see figure 8.6a). The reference signal is filtered to a frequency of $2.5Hz$ (about 22.4 m spatial resolution) and FIT with the random values of d from PDF (calculated from the reference POST signal) is applied to reconstruct the sub-filter part of the dataset. It is important to note that FIT can be carried out in time by replacing the spatial variable x in equations (7.1) to (7.6) with time. The frequency spectra for the reference POST, filtered POST and FIT velocity dataset are shown in figure 8.6a. Once again, it is observed that the approach with random d follows the inertial-range scaling closer than the other two approaches.

Differences in the observed spectra are quantified as follows. Under the local isotropy assumption and within the validity of the Taylor's hypothesis, the energy spectra in the inertial range can be converted to the frequency spectra, see Ref. [126]

$$S_{th} = C_1 \left(\frac{U}{2\pi} \right)^{2/3} \epsilon^{2/3} f^{-5/3}, \quad (8.2)$$

where the constant $C_1 \approx 0.49$, $U = 55ms^{-1}$ is the true air speed of the aircraft and ϵ is the turbulence kinetic energy dissipation rate. The value of ϵ can be estimated from the linear-least-squares fit procedure applied in a certain range of frequencies. In the present case, $f = 0.1Hz - 2.0Hz$ is used and calculated $\epsilon = 4.1306 \times 10^{-4} \text{ m}^2/\text{s}^3$. Deviations of the spectra reconstructed with FIT from the inertial-range scaling are

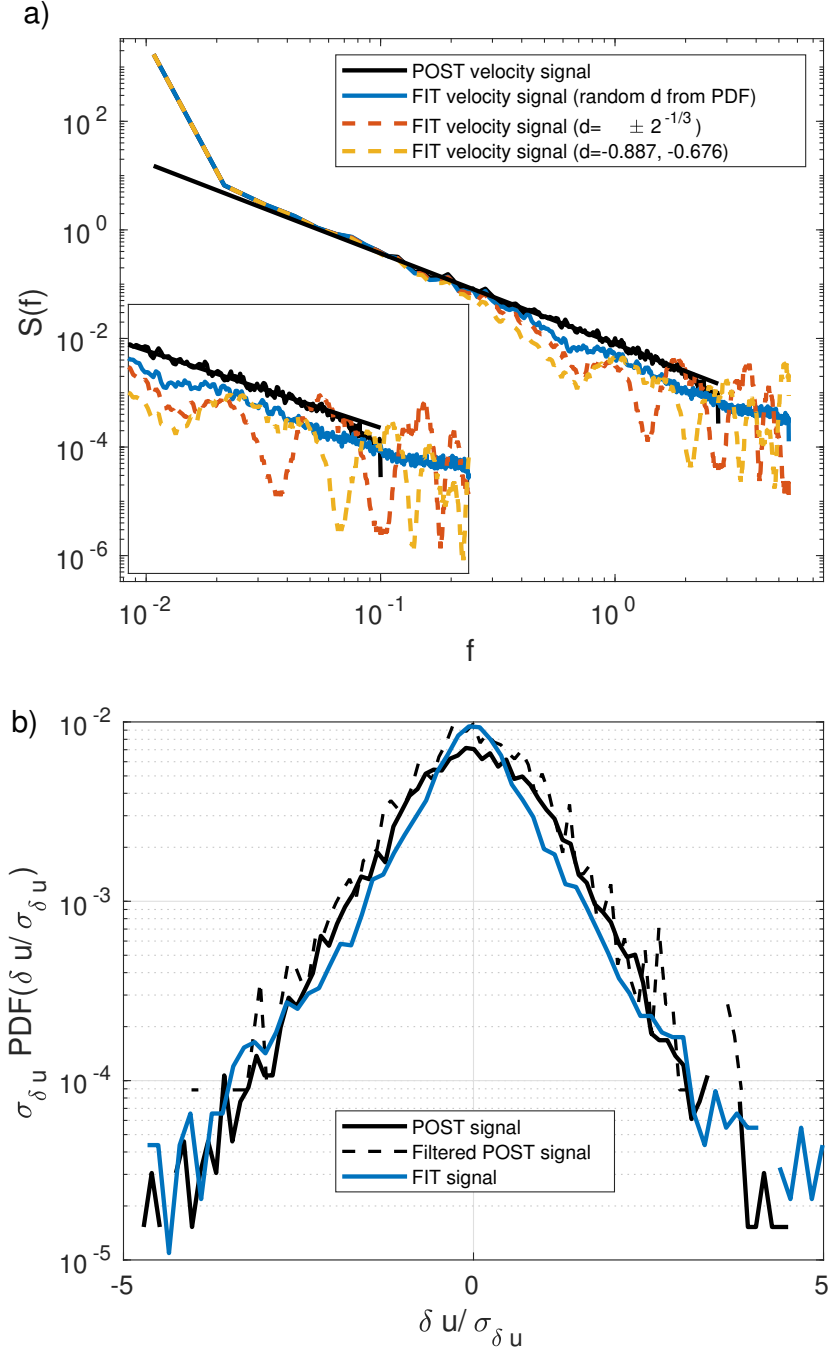


Figure 8.6: (a) Longitudinal energy spectra of POST airborne data and FIT reconstructed signal with constant stretching parameter $d = \pm 2^{-1/3}$, $d = -0.887$ and $d = -0.676$ and random stretching parameters from its PDF. (b) PDFs of velocity increments for POST, filtered POST and FIT signals with random values of d .

quantified with δ_S defined as

$$\delta_S = \left[\frac{\int_{f_{cut}}^{\infty} \langle (S_{th} - S(f))^2 \rangle df}{\int_{f_{cut}}^{\infty} \langle S_{th}^2 \rangle df} \right]^{0.5} \quad (8.3)$$

where $S(f)$ is the FIT frequency spectrum and $f_{cut} = 2.5Hz$ is the cut-off frequency, i.e. the frequency at which the fractal reconstruction is initiated. The following values of δ_S is obtained

$$\begin{aligned}\delta_S &= 0.033 && \text{for FIT procedure with } d = \pm 2^{-1/3} \\ \delta_S &= 0.049 && \text{for FIT procedure with } d = -0.887, -0.676 \\ \delta_S &= 0.026 && \text{for FIT procedure with random } d\end{aligned}$$

It follows that the FIT model with random values of d reproduces the inertial range scaling with the smallest error. Next, I compare the PDF of velocity increments for POST reference data, filtered POST and FIT data with random values of d in figure 8.6b. The velocity increments were calculated as $u(t + \tau) - u(t)$ with $\tau = 0.1$ s. The PDF of velocity increments for POST reference data and FIT data agree reasonably well.

8.3 3-D fractal interpolation of LES

Next, fractal interpolation of three components of velocity in 3D using the random values of d (from the PDF shown in figure 7.10) is performed. Each velocity component is filtered with the decimate function (described in section 7.4.1) to a grid resolution of 20 m from its initial 5 m grid resolution to remove the smallest scales spuriously damped due to numerical diffusion. Then, I perform a 3-D fractal reconstruction of inertial-range scales to a grid resolution of 5 m (i.e. two reconstruction steps), as described in section 7.1 without considering any correlations which might exist between the directions. It is important to note that the filtering operation (i.e. decimate function) is performed on 1-D intersections of the velocity fields (i.e. separately along x -, y - and z - directions) analogous to the way FIT is carried out in 3-D.

Figure 8.7 presents contour plots of the longitudinal u velocity component at $z = 595$ m for filtered LES and FIT-reconstructed field. The addition of inertial-range sub-grid structures in FIT velocity is clearly visible. Energy spectra of this field are presented in Fig. 8.8 and compared with the two other FIT approaches with constant d . The deviations from $-5/3$ scaling are calculated with a formula analogous to Eq. (8.3)

$$\delta_E = \left[\frac{\int_{k_{cut}}^{\infty} \langle (E_{th} - E_{11}(k))^2 \rangle dk}{\int_{k_{cut}}^{\infty} \langle E_{th}^2 \rangle dk} \right]^{0.5}, \quad (8.4)$$

where E_{th} is described by

$$E_{th} = C_1 \epsilon^{2/3} k^{-5/3}. \quad (8.5)$$

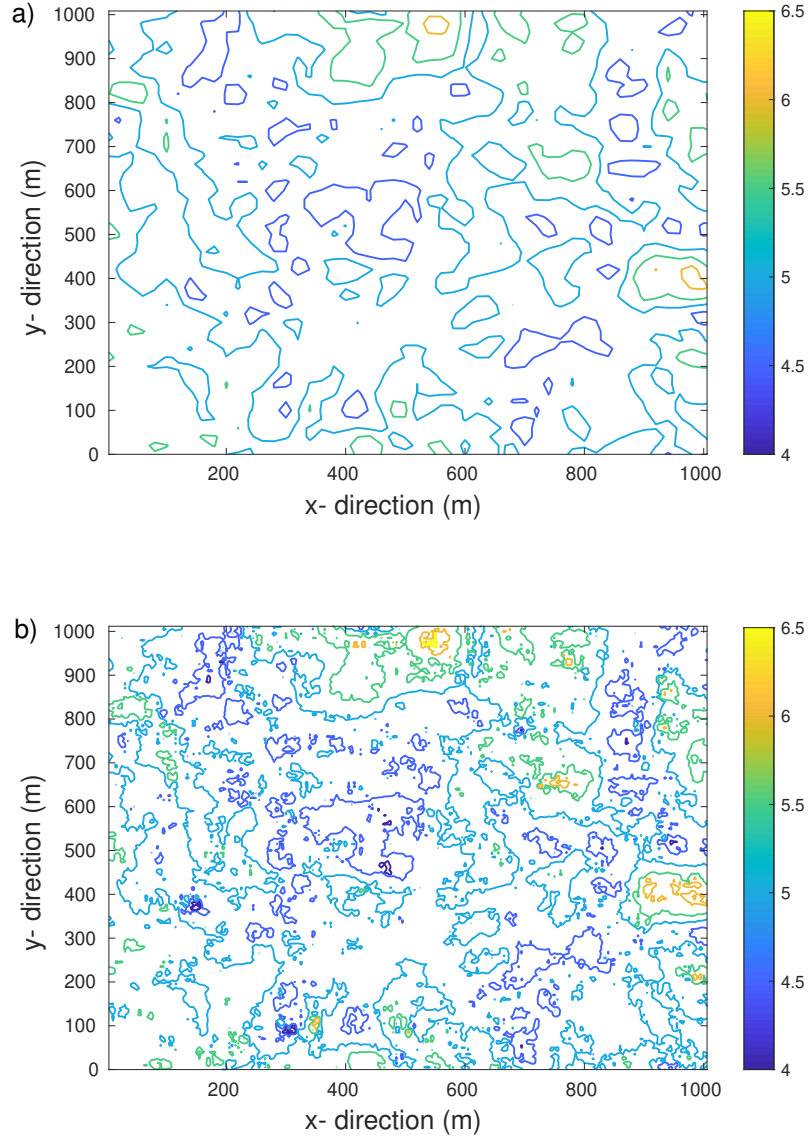


Figure 8.7: Contour plot of u velocity field (a) filtered LES velocity field, (b) velocity field of LES with FIT.

With the fitting range $k = 0.019\text{m}^{-1} - 0.044\text{m}^{-1}$, the value $\epsilon = 5.0299 \times 10^{-5} \text{ m}^2/\text{s}^3$ is estimated.

The obtained results read

$\delta_E = 0.40$	for FIT procedure with $d = \pm 2^{-1/3}$,
$\delta_E = 0.52$	for FIT procedure with $d = -0.887, -0.676$,
$\delta_E = 0.28$	for FIT procedure with random d .

Here again, FIT with random values of d shows the best agreement with the $-5/3$

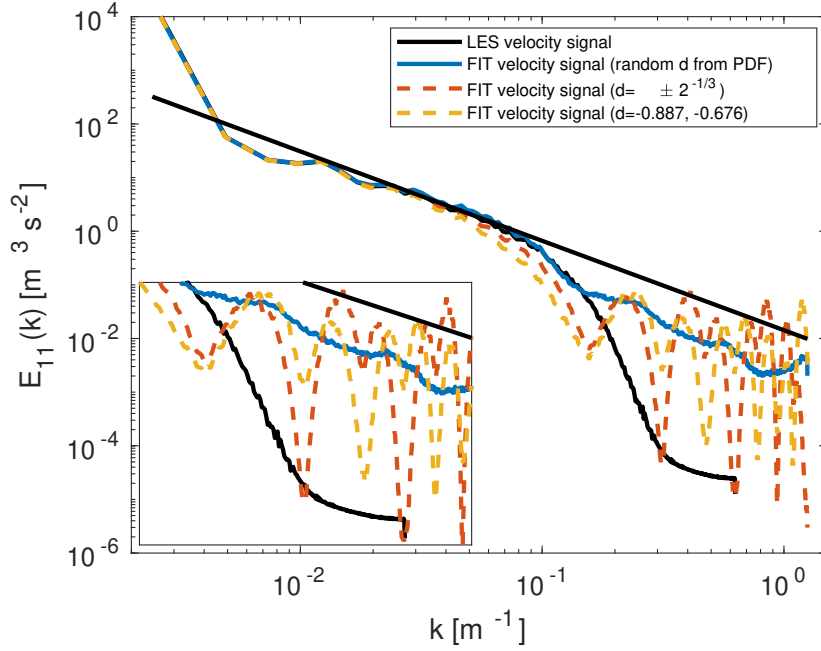


Figure 8.8: Longitudinal energy spectra of LES velocity field and FIT-reconstructed field with a constant stretching parameter $d = \pm 2^{-1/3}$, $d = -0.88, -0.676$ and random stretching parameters from PDF.

inertial-range scaling.

Figure 8.9 presents the PDFs of velocity increments for u , v and w components, separately, calculated at the distance $r = 5m$ at horizontal plane $z = 595m$. LES (without filtering) with the FIT-reconstructed field is compared. As it is seen, LES results are closer to Gaussian, while PDFs calculated from the FIT-reconstructed field have the exponential tails. This could be explained by the fact that the smallest resolved scales of LES are spuriously damped due to numerical diffusion, hence, the inertial-range intermittency is not reproduced by LES velocity field.

As reported by Ref. [120], a limitation of the fractal model is that the sub-grid scale velocity field is not divergence free due to the loss of the correlation between directions. To investigate this issue, the error in mass conservation at different reconstruction steps is calculated. For this, the following formula is used

$$\delta_{\nabla \mathbf{u}} = \sqrt{\frac{1}{n \cdot m \cdot p} \sum_{i=1}^n \sum_{j=1}^m \sum_{k=1}^p (\nabla \cdot \mathbf{u})_{ijk}^2}. \quad (8.6)$$

where n, m, p is the number of grid points in x , y and z directions, respectively. The divergence of velocity field is calculated with the central difference scheme. Additionally, the error in mass conservation is characterized by the quantity $|\max(\nabla \cdot$

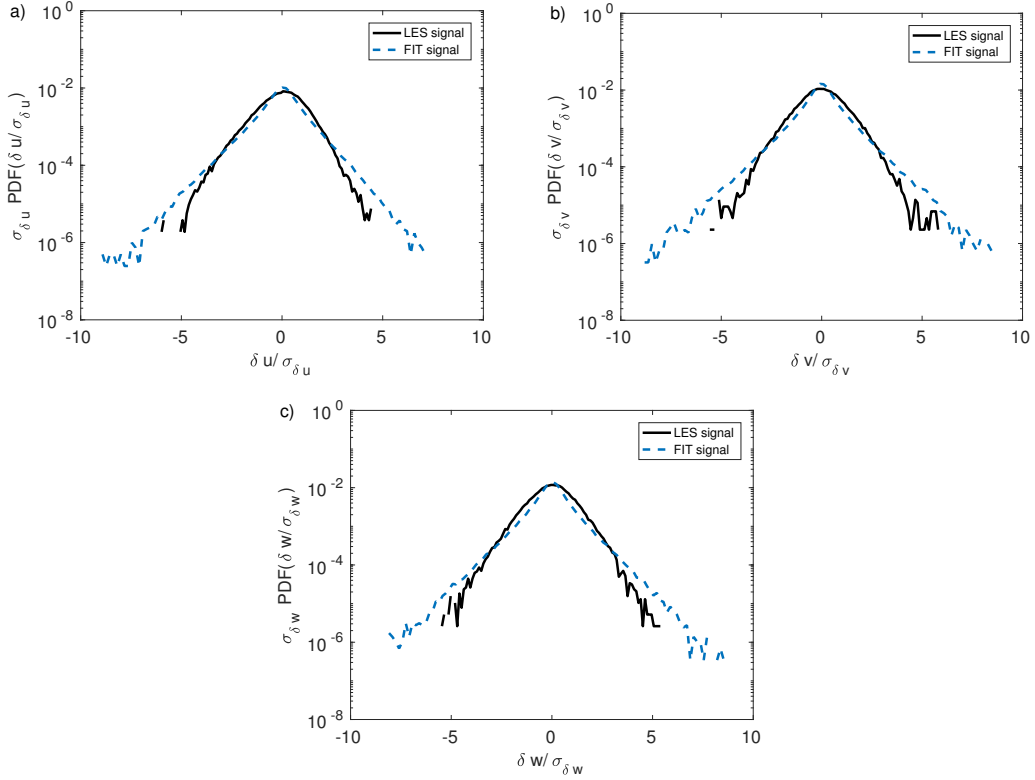


Figure 8.9: (a) PDFs of LES and FIT velocity increments δu , (b) PDFs of LES and FIT velocity increments δv , (c) PDFs of LES and FIT velocity increments δw . FIT with random d was applied.

$\mathbf{u}) - \min(|\nabla \cdot \mathbf{u}|)$. LES field is filtered to $k_{cut} = 0.150, 0.075$ and $0.037m^{-1}$, which corresponds to the grid resolution of approximately 10, 20 and 40m, respectively. Next, the signal is reconstructed to the resolution 5m, which means that one FIT reconstruction step was applied to the signal with $k_{cut} = 0.150m^{-1}$, using two steps to obtain the signal with $k_{cut} = 0.075m^{-1}$ and three steps to obtain the signal with $0.037m^{-1}$. Results are presented in Tab. 8.1.

In theory, $\delta_{\nabla \mathbf{u}}$ should be zero but due to numerical errors, the divergence of filtered LES velocity fields could be non-zero. As seen in Tab. 8.1, there is a difference in $\delta_{\nabla \mathbf{u}}$ of two orders of magnitude between LES and the filtered LES without FIT reconstruction when the decimate function is used. In spite of this, filtered velocity fields are commonly used to do *a priori* tests to estimate e.g. an effect of SGS models on particle statistics [56, 106, 107]. Each FIT reconstruction step increases the error in mass conservation, however, after two steps $\delta_{\nabla \mathbf{u}}$ is still of the same order of magnitude as the error of filtered LES without reconstruction, at least for the FIT method with random d and for FIT with constant $d = -0.887, -0.676$.

Method	k_{cut} [m ⁻¹]	Number of reconstruction steps	$\delta_{\nabla \mathbf{u}}$	$ max(\nabla \cdot \mathbf{u}) - min(\nabla \cdot \mathbf{u}) $
LES - no filtering	0.3	0	0.00003	0.00051
Filtered LES - no FIT	0.037	0	0.0036	0.0554
FIT with constant $d = \pm 2^{-1/3}$	0.150	1	0.0106	0.2023
	0.075	2	0.0142	0.4379
	0.037	3	0.0218	0.7189
FIT with constant $d = -0.887, -0.676$	0.150	1	0.0066	0.1395
	0.075	2	0.0097	0.2849
	0.037	3	0.0156	0.6322
FIT with random values of d from PDF	0.150	1	0.0064	0.1253
	0.075	2	0.0087	0.2962
	0.037	3	0.0105	0.6052

Table 8.1: Values of $\delta_{\nabla \mathbf{u}}$ for different k_{cut} and different fields.

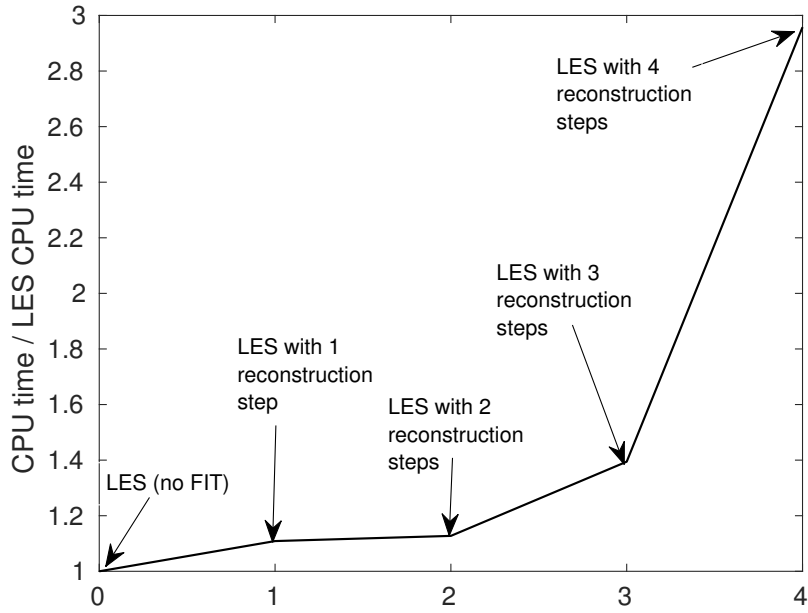


Figure 8.10: Additional computational time required for fractal interpolation technique.

The difference between the maximum and minimum of the divergence of the velocity fields is seen to be one order of magnitude larger if all FIT models are compared with filtered LES. Of all FIT approaches, the new proposal with random values of d gives the smallest value of $\delta_{\nabla \mathbf{u}}$ and $|max(\nabla \cdot \mathbf{u}) - min(\nabla \cdot \mathbf{u})|$. Based on this result, it

can be suggested that one or two iteration steps of FIT to LES velocity field should not be exceeded to keep the error in mass conservation at an acceptable level.

Next, the computational cost of the FIT procedure applied to three velocity components in 3D space is investigated. For this, one to four reconstruction steps are performed. As presented in Fig. 8.10, the computational cost (CPU time) of one, two or even three FIT reconstruction steps is small compared to the time needed for LES to resolve large scale features. This shows that the newly proposed fractal model is not only able to reproduce inertial-range eddies but is also computationally efficient.

Chapter 9

Fractal subgrid scale model - applications

This chapter outlines possible applications for the fractal subgrid scale model described and analyzed in chapter 8. It explains how the resolved stresses for a test filter and residual kinetic energy can be reconstructed with the fractal subgrid model, by performing an *a priori* LES test. Furthermore, the fractal subgrid scale model will be applied to the reconstruction of inertial-range subgrid scales for the Lagrangian tracking of passive tracers in LES velocity field. In perspective, the model can be coupled with the super-droplet method of Ref. [125].

9.1 Reconstructing resolved stresses for a test filter and residual kinetic energy

Large eddy simulation technique is commonly used for the calculations of turbulent flows in both simple and complex configurations [25, 90, 105]. In LES, the unresolved scales of motion act on the resolved velocity field as new stresses (called subgrid stresses), which need to be modeled [104]. For better understanding, consider an incompressible turbulent flow, which obeys the Navier-Stokes equations in a domain Ω , bounded by $\delta\Omega$. If a spatial filter of characteristic width Δ is applied to the real velocity field $u_i(\mathbf{x}, t)$, the filtered velocity field $\tilde{u}_i(\mathbf{x}, t)$ obtained obeys the filtered Navier-Stokes equations

$$\frac{\partial \tilde{u}_i}{\partial x_i} = 0, \quad (9.1)$$

$$\frac{\partial \tilde{u}_i}{\partial t} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \tilde{p}}{\partial x_j} + \nu \nabla^2 \tilde{u}_i - \frac{\partial \tau_{ij}}{\partial x_j}, \quad (9.2)$$

where the subgrid stress tensor is given by

$$\tau_{ij} = \widetilde{u_i u_j} - \widetilde{u_i} \widetilde{u_j} \quad (9.3)$$

and the residual kinetic energy is

$$k_r \equiv \frac{1}{2} \tau_{ii}^R = \frac{1}{2} [\widetilde{u_i^2} - \widetilde{u_i}^2]. \quad (9.4)$$

As seen, equations (9.1) - (9.2) can be solved for the velocity field $\widetilde{u_i}(\mathbf{x}, t)$ if a suitable model for the subgrid scale stresses is provided [109]. Reconstruction of subgrid-scale motions is also useful for LES of particle dispersion in turbulent flows since only about 80% or less of the turbulent kinetic energy is resolved. To validate whether the fractal reconstruction of subgrid velocity can recover energy of subgrid stresses, an *a priori* LES test is performed with the LES dataset of stratocumulus-top boundary layer (described in section 7.3.2). Our definition of *a priori* test in this section is quite different from its usual definition, in which DNS velocity field is filtered to validate LES closures [25, 109]. For this analysis, the fractal subgrid scale model is validated by applying a top-hat filter (test filter) to the LES velocity field $\widetilde{\mathbf{u}}$ to obtain a coarser velocity field $\widehat{\mathbf{u}}$. The coarser field $\widehat{\mathbf{u}}$ should satisfy the Navier-Stokes equations as in equations (9.1) and (9.2) and its corresponding subgrid-scale stress T_{ij} is [43]

$$T_{ij} = \widehat{\widetilde{u_i u_j}} - \widehat{\widetilde{u_i}} \widehat{\widetilde{u_j}}. \quad (9.5)$$

Since LES velocity fields do not contain sub-grid scales, the subgrid-scale stress T_{ij} can not be reproduced. The resolved stress L_{ij} for the test filter is defined as

$$L_{ij} = \widehat{\widetilde{u_i} \widetilde{u_j}} - \widehat{\widetilde{u_i}} \widehat{\widetilde{u_j}} \quad (9.6)$$

represent the contribution of scales whose length is between the LES grid width and the coarser LES grid width to the Reynolds stress [43]. For this type of *a priori* test, the resolved stress L_{ij} for the test filter can be reconstructed with the fractal subgrid scale model. This type of validation is applied because the fractal model (described in chapter 8) is only capable of reproducing scales in the inertial range of the energy spectrum, in which the PDFs of the stretching parameter are self-similar. Most DNS are performed at low or moderate Reynolds' number, which have short inertial range energy spectrum (as seen in section 5.1.1). For this reason, it is difficult to access the ability of the fractal subgrid model to reproduce inertial range scales using available low-Reynolds number DNS velocity fields.

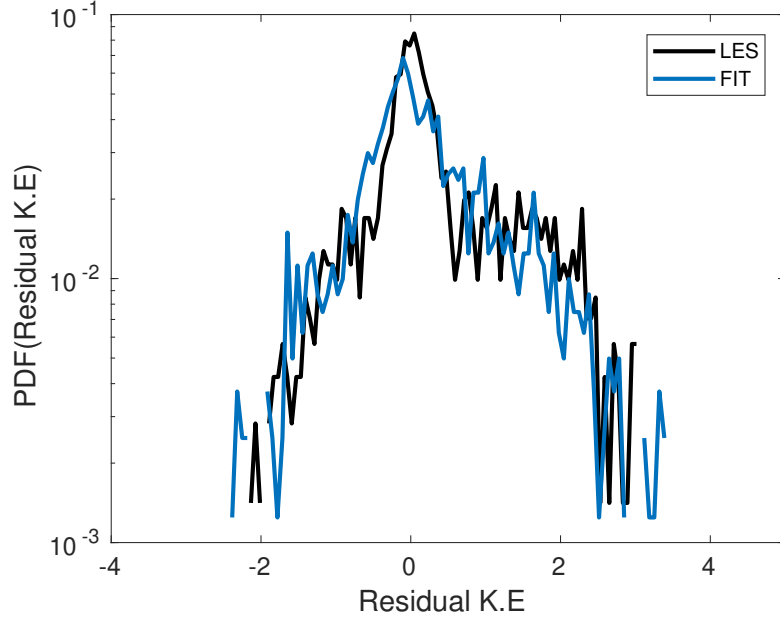


Figure 9.1: PDF of the residual kinetic energy for reference LES and filtered LES with FIT in the in-cloud region at $20 \text{ m} \leq z \leq 650 \text{ m}$.

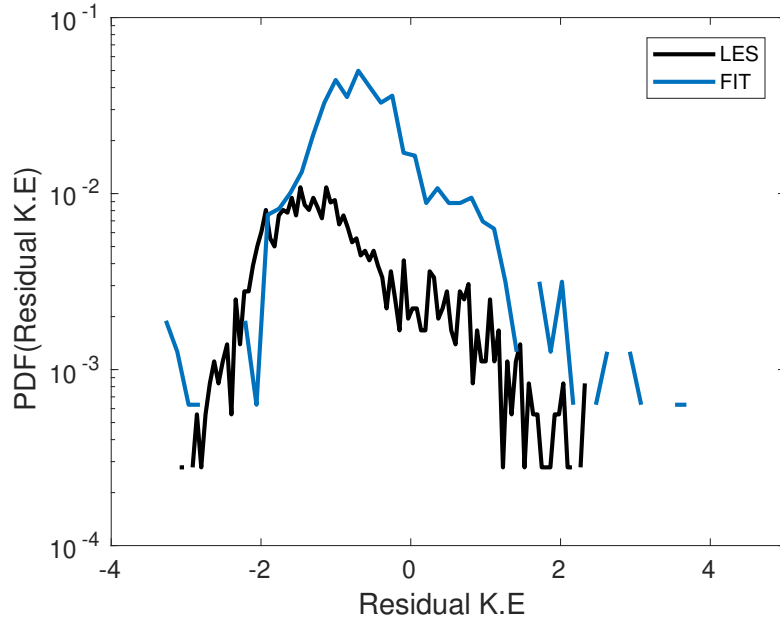


Figure 9.2: PDF of the residual kinetic energy for reference LES and filtered LES with FIT above the cloud-top region at $700 \text{ m} \leq z \leq 1200 \text{ m}$.

Next, *a priori* LES testing is performed as follows. First, LES velocity fields from stratocumulus-top boundary layer simulation (described in section 7.3.2) were

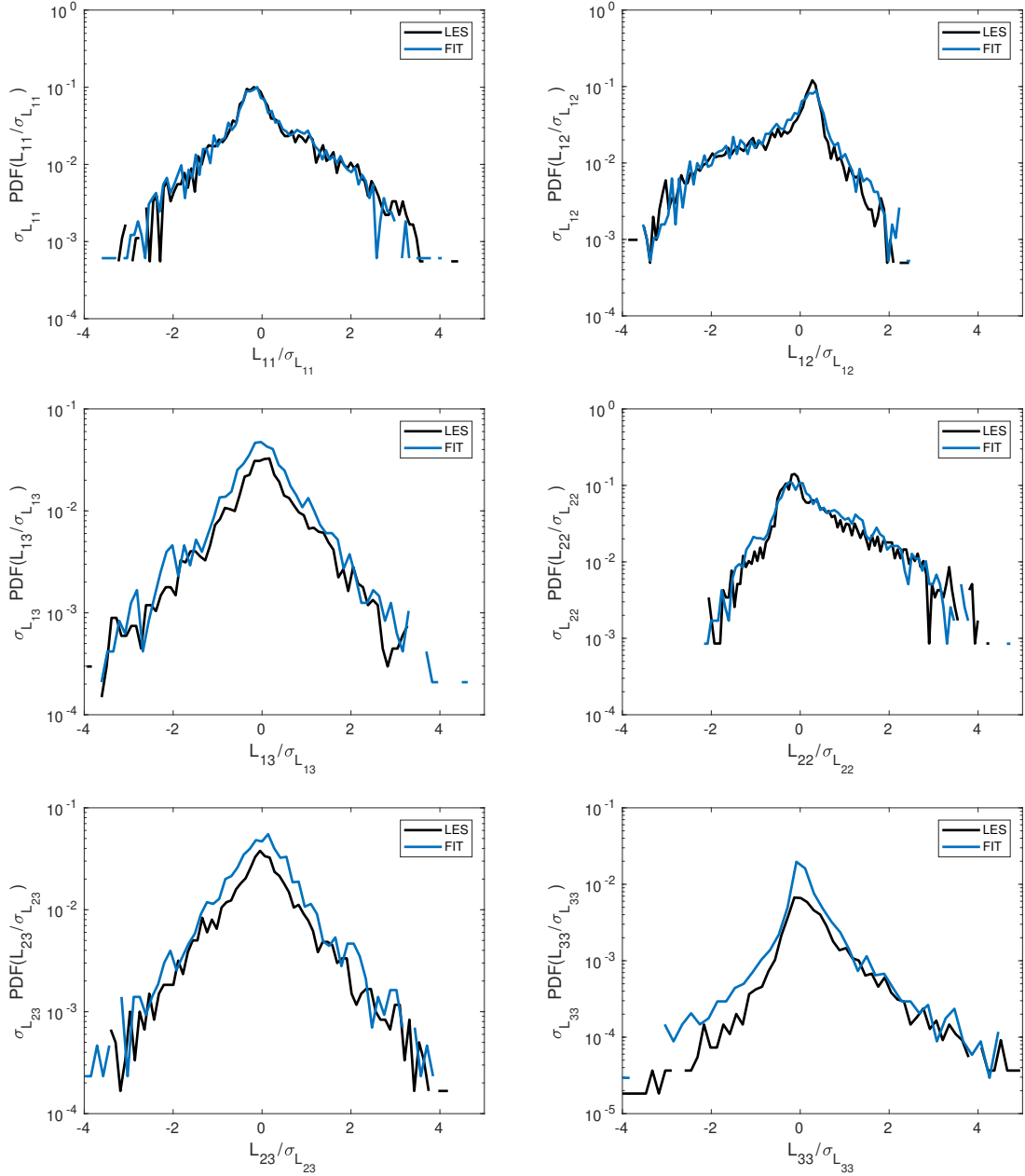


Figure 9.3: PDF of resolved stresses L_{11} , L_{12} , L_{13} , L_{22} , L_{23} and L_{33} for reference LES and filtered LES with FIT in the in-cloud region at $20 \text{ m} \leq z \leq 650 \text{ m}$.

filtered (using the decimate function described in section 7.4.1) to a grid resolution of 40 m from its 5 m resolution to remove the smallest scales spuriously damped due to numerical diffusion. This filtered LES with grid resolution of 40 m will be referred to as the reference LES velocity fields. Second, the LES velocity fields were filtered again to a grid resolution of 160 m from its 5 m resolution, which will be called filtered LES velocity field. The fractal interpolation procedure (as described in section 7.1

with random stretching parameters) were performed on the filtered LES velocity field using two reconstruction steps to obtain FIT velocity fields. Lastly, the PDF of the resolved stresses L_{ij} (using equation 9.6) computed with the reference LES velocity fields were compared with the PDF of the resolved stresses L_{ij}^{FIT} computed with FIT velocity fields. As described in section 7.3.2 (see figure 7.6), the cloud-top region is at $z \sim 700$ m. Below this region (also called in-cloud region i.e. $20 \text{ m} \leq z \leq 650 \text{ m}$), the turbulence intensity is high and turbulence is close to isotropic while above the cloud-top region (i.e. $700 \text{ m} \leq z \leq 1200 \text{ m}$), the turbulence intensity is low and turbulence is strongly inhomogeneous. Analyses for these regions were performed separately. Figure 9.1 shows the PDF of the residual kinetic energy for the reference LES and filtered LES with FIT in the in-cloud region. A good agreement is observed between both profiles. The same is observed in figure 9.3, which shows the PDFs of all resolved stresses L_{ij} for the reference LES and filtered LES with FIT in the in-cloud region. However, there are deviations, due to turbulence anisotropy, between the PDFs of reference LES and filtered LES with FIT above the cloud-top region as seen in figure 9.2. FIT adds too much fluctuation in this stably stratified, weakly-turbulent region (above the cloud-top), causing these deviations.

9.2 Reconstructing inertial range scales for the Super-droplet Method - preliminary test

Shima et al. (2009) [125] proposed a Lagrangian technique for the simulation of cloud microphysics, named the super-droplet method (SDM). The super-droplet method features an efficient Monte-Carlo type solver for droplet coalescence. Each super-droplet for which computations are made represents a multiplicity of real-world droplets with the same position, radius and composition. Two mutually coupled components form the framework for this method. These are the Eulerian fluid flow solver to calculate turbulent velocity field and a Lagrangian particle-tracking of physical coordinates and physicochemical properties of droplets in the turbulent flow. The condensation and evaporation of water on the super-droplets is represented as the source or sink of water vapour and heat, which the Eulerian component feeds on. The Lagrangian component needs the fluid velocity field in order to update both the positions of the super-droplets and the thermodynamic fields, which is needed to compute condensational growth and evaporation rates [14, 35, 125]. The motion of each super-droplet is governed by

$$\mathbf{v}_i(t) = \mathbf{U}(\mathbf{x}_i, t) - \hat{z}v_\infty(R_i), \quad \frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i, \quad (9.7)$$

where $\mathbf{U}(\mathbf{x}_i, t)$ is the fluid velocity field at the super-droplet position $\mathbf{x}_i$ and $v_\infty(R_i)$ is the terminal velocity of the super-droplet with radius R_i .

To accurately predict super-droplets' positions and other thermodynamic fields, the model spatial resolution has to be high enough to resolve at least large turbulent scales and needs to include appropriate contribution of subgrid scales [46]. Unfortunately, due to high-Re of atmospheric flows, Lagrangian cloud models [13, 115, 125] exclude the latter to the best of the author's knowledge. To account for the effect of the subgrid scales on super-droplet motion and growth/evaporation, Grabowski and Abade (2017) [46] developed an eddy-hopping model, in which they showed that (based on their model) for spatial scales larger than 10 m, the impact of turbulence is high. The eddy-hopping mechanism, suggested by Cooper (1989) [31], describes an idea that cloud droplets experience different growth histories due to the local fluctuation of the supersaturation as they hop from one eddy to the other. They showed that the representation of the eddy-hopping mechanism can be included in the Lagrangian LES cloud model and may lead to an improved representation of cloud collision-coalescence [1, 46]. The fractal subgrid scale model can also be used as an alternative of the eddy-hopping model, which did not include the effects due to the spatial structure of sub-grid fields, e.g. the non-Gaussianity of velocity increments due to flow intermittency.

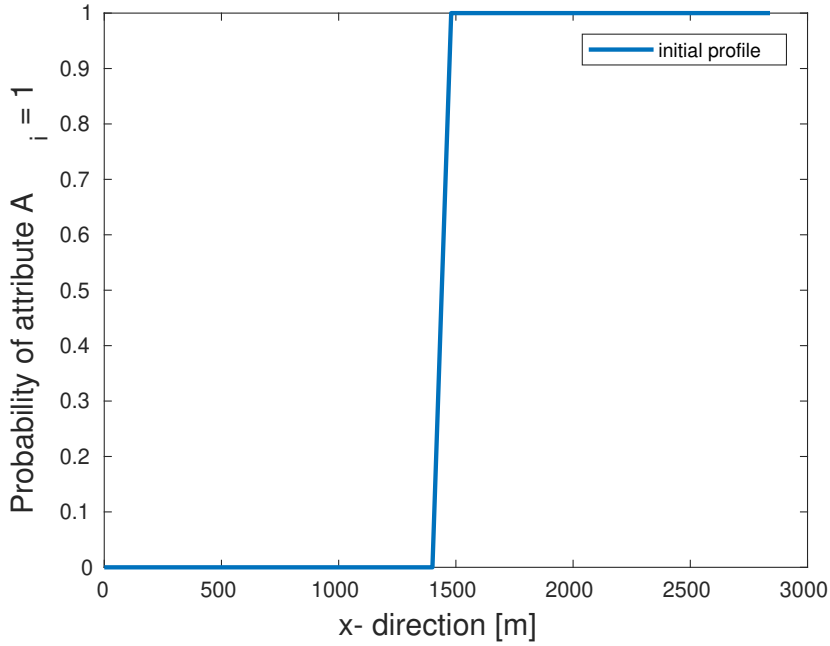
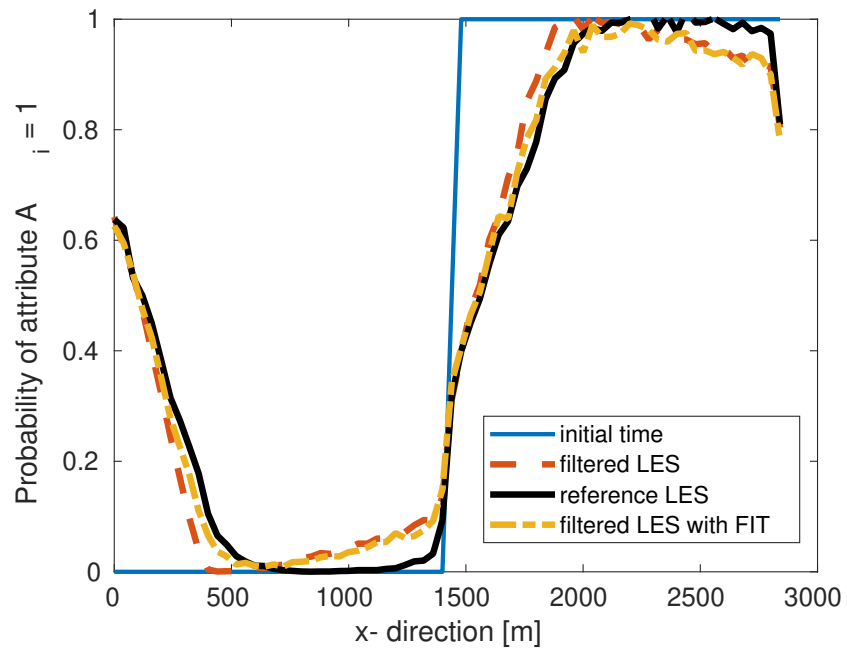


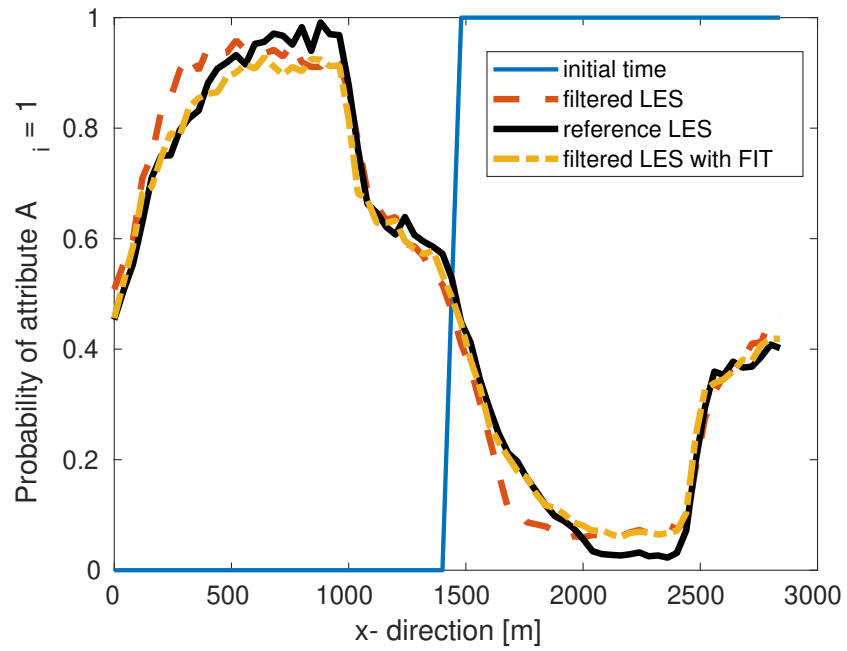
Figure 9.4: The initial profile of the attribute probability $A_i = 1$ in the x - direction, averaged in y - and z - directions.

As a preliminary test for the fractal sub-grid scale model, Lagrangian tracking of super-droplets in a frozen LES field is performed. The configuration of the LES field (of stratocumulus-top boundary layer) is described in section 7.3.2. For this test, the terminal velocity of each super-droplet is assumed to be very small as compared to fluid velocity $\mathbf{U}(\mathbf{x}_i, t)$ (i.e. $v_\infty(R_i) \approx 0$) since cloud droplets of radii $1\mu m \leq R_i \leq 30\mu m$ have approximately zero terminal velocities. This assumption is valid when the super-droplets sizes and the energy dissipation rate are sufficiently small [147] such as in small cumulus or stratiform clouds. It is also important to note that the purpose of this analysis is not to compute explicitly any of the cloud microphysical properties as done in Shima et al (2009) [125], however, it is obvious that the motion of each super-droplet influences the accuracy of the model for these microphysical properties (such as the supersaturation). For simplicity, our super-droplets have only one attribute denoted as A_i . For this case, I assume that the attribute of each super-droplet does not change in time. The computational domain is partitioned equally into two sub-domains in the x - direction. Super-droplets were initially positioned randomly within the domain. Droplets in the first half of domain have attribute $A_i = 0$ while the remaining ones were placed in the other half with attribute $A_i = 1$ (see figure 9.4). The initial positions of particles in x -, y - and z - directions are chosen randomly from the uniform distribution. A total of 300,000 super-droplets were used for this analysis, such that on average, two super-droplets are placed in each LES computational cell.

(a)



(b)



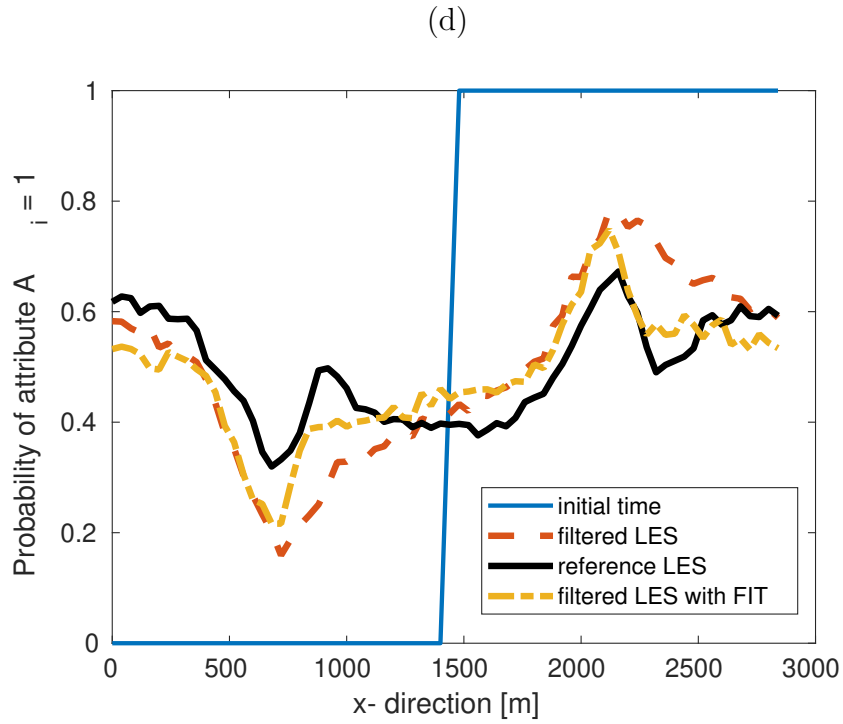
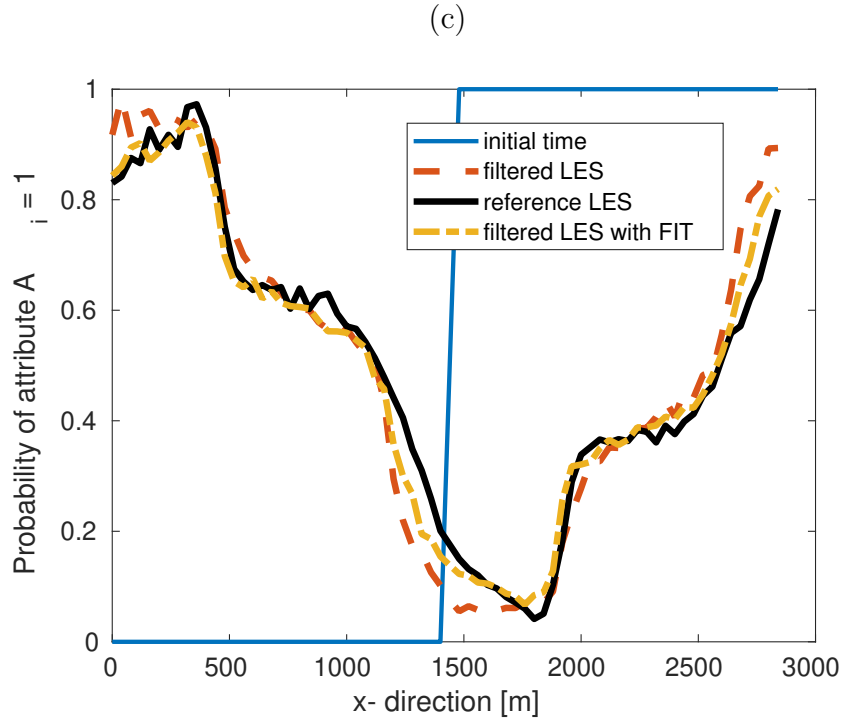
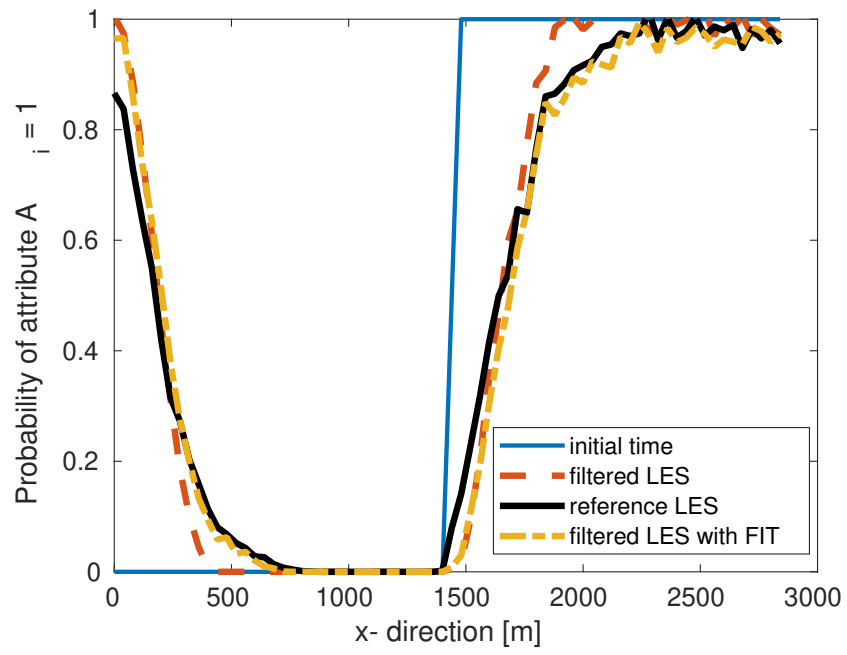
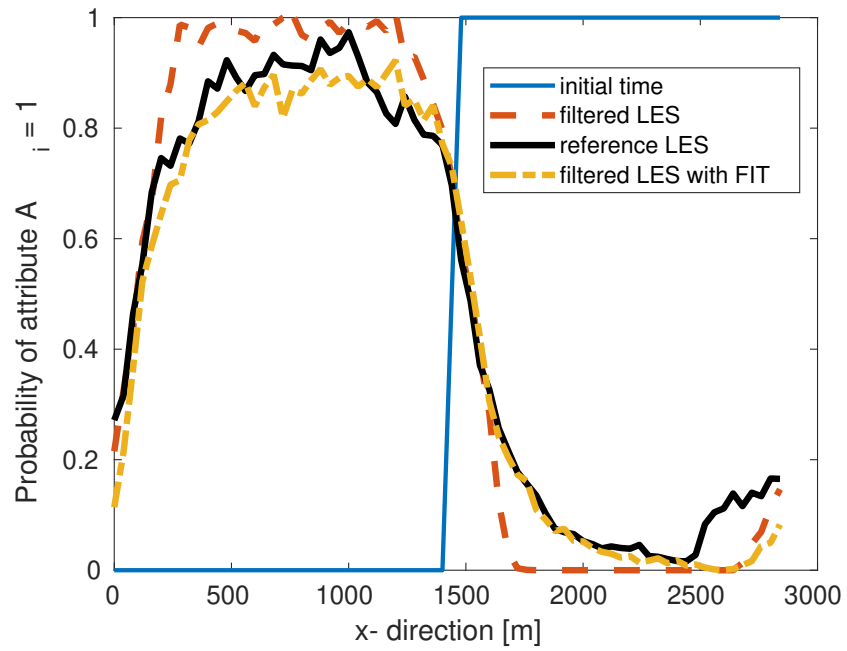


Figure 9.5: The attribute probability $A_i = 1$ in the x - direction, averaged over y - and z - directions in the whole domain at (a) $t = 30$ minutes (b) $t = 60$ minutes (c) 90 minutes (d) 120 minutes of simulation time.

(a)



(b)



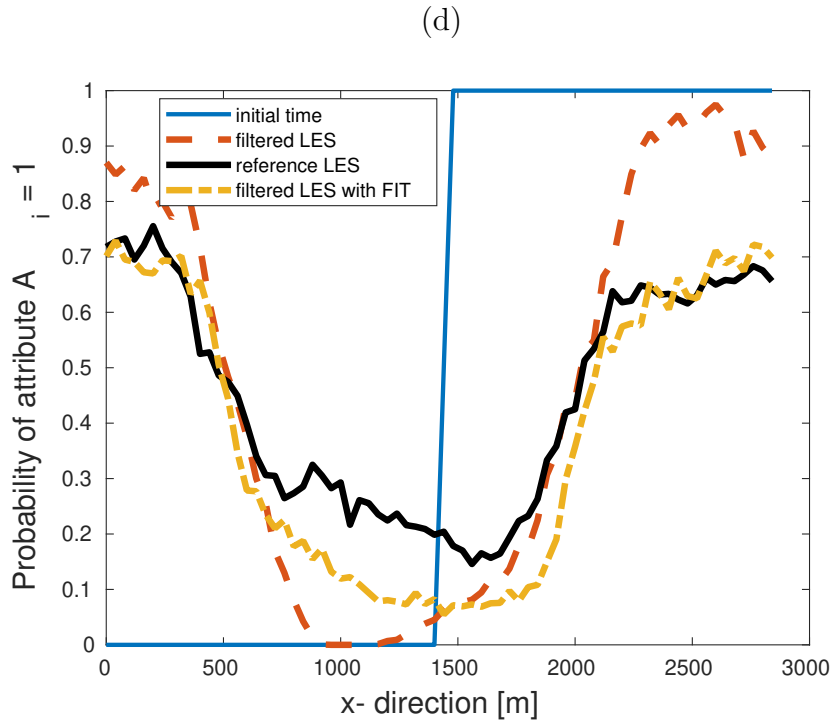
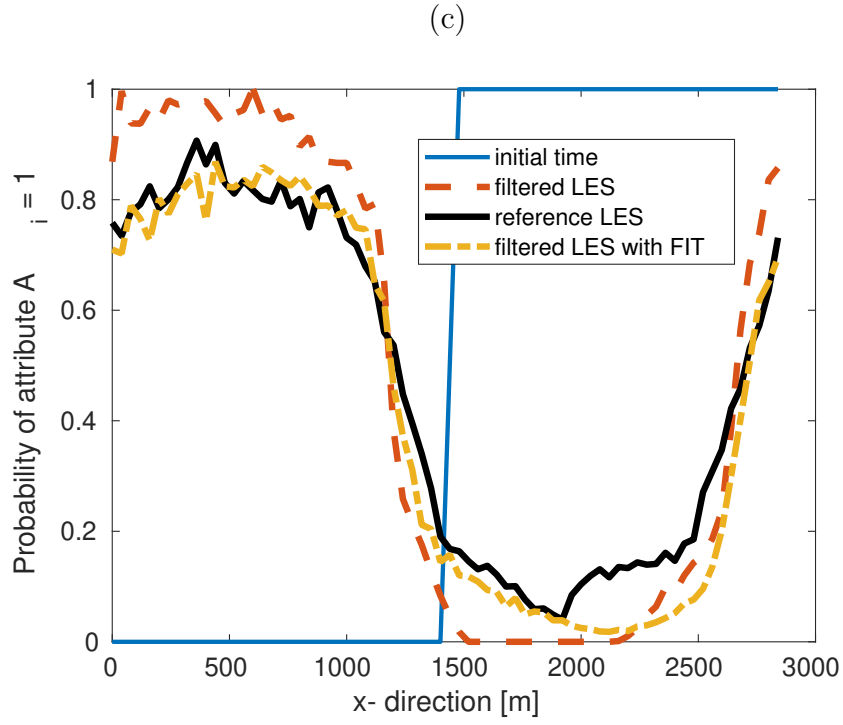


Figure 9.6: The attribute probability $A_i = 1$ in the x - direction, averaged over y - and z - directions in the in-cloud region only at (a) $t = 30$ minutes (b) $t = 60$ minutes (c) 90 minutes (d) 120 minutes of simulation time.

Next, the trajectory of each super-droplet is solved using equation (9.7) and $v_\infty = 0$ in three different fluid velocity fields: reference LES velocity field, filtered LES velocity field and filtered LES with FIT. The resolution of these velocity fields are the same as those used in the computation of residual kinetic energy and Leonard stresses in section 9.1, that is the reference LES velocity field and filtered LES with FIT have a resolution of 40 m while the filtered LES velocity field have 160 m grid resolution. The dynamics of LES as written in equations (9.1) - (9.2) is not solved for, hence, LES is treated as a “kinematic model” with no variation in time. The dynamics of LES with the fractal subgrid scale model is left for future work. Trilinear interpolation was used to calculate the velocity of the fluid $\mathbf{U}(\mathbf{x}_i)$ at each super-droplet position $\mathbf{x}_i$ and the particle motion is periodic in x - and y - directions and bounces-back in z - direction. The simulation time step is chosen such that the maximum value of Courant-Friedrichs-Lewy condition throughout the domain is 0.5 and the simulation period is 120 minutes.

Figure 9.5 shows the probability of having attribute $A_i = 1$ as a function of x , averaged over y - and z - directions at $t = 30$ minutes, $t = 60$ minutes, $t = 90$ minutes and $t = 120$ minutes. We see the initial profile of the attribute probability $A_i = 1$ changing shape as super-droplets follow the flow. At about $t = 30$ minutes (see figure 9.5a), slight deviation is observed between the probability of attribute $A_i = 1$ for the reference LES and coarse LES. At the final time (for $t = 120$ minutes), the probability of attribute $A_i = 1$ for the filtered LES with FIT agrees somewhat better with the reference LES than the coarse LES. Since it was shown previously in section 9.1 that the FIT gives better results in the isotropic in-cloud region (i.e. $20 \text{ m} \leq z \leq 650 \text{ m}$), this comparison is done for particles placed in this region only, see figure 9.6. We see a better agreement between the probability of attribute $A_i = 1$ for the filtered LES with FIT and reference LES because the inertial-range scales (that were filtered out) have been replaced by fractal reconstruction. It is argued that this analysis, although simplified, allows to draw a conclusion that FIT can be used to improve the resolution of LES velocity field for the simulation of cloud microphysics. The improvement is expected to exist especially in the in-cloud region where turbulence is approximately isotropic.

Chapter 10

Comprehensive summary and outlook

10.1 Summary

In this thesis, the focus was on the analysis and numerical reconstruction of small-scale turbulence. This work is divided into two parts:

In the first part of the thesis, I investigated the scaling of energy spectra of turbulent flows in atmospheric configurations and different methods for TKE dissipation rate retrieval from $1D$ intersections of the flow domain. Data from numerical experiments in two different configurations were studied. These are: the stratocumulus cloud-top simulations and free convective boundary layer. In such experiments high Re numbers observed in nature could not be reached, however, it is argued that model assumptions can be tested and conclusions applicable also to "real-world" flows can be drawn. I observed that the investigated cases are influenced mainly by buoyancy effects which causes deviations from the Kolmogorov scaling. This, in turn, results in errors of TKE dissipation rate retrieval based on local isotropy assumption. In both considered flow cases, the longitudinal spectra of horizontal velocity components $E_{11}(k_1)$ and $E_{22}(k_2)$ compare quite well with the Kolmogorov scaling over a certain range of wavenumbers, whereas it is not the case for the transverse spectra. The $1D$ spectra of the vertical component show $-5/3$ scaling range, however, the constant α' is larger than the isotropic value. As a result, TKE dissipation rate estimates from u , v and w velocity component differ, which withstands the local isotropy assumption. It was shown that the estimates in the upper part of the cloud and the boundary layer, where the buoyancy flux is minimum and stable stratification strongly hinders vertical motions, are subject to significant errors. I investigated different methods of TKE dissipation rate retrieval, including the approaches based on the number of crossings

per length proposed in Ref. [144]. Both methods are devised for the case where a measured velocity signals have a spectral cut-off. The first method uses inertial-range arguments and provides scaling of N_L in this range. From results presented in Section 5.1, it was concluded that the performance of this approach is comparable with the standard spectral retrieval methods. The second method proposed in Ref. [144] is based on the recovery of the missing part of the spectrum, i.e. the part with k higher than the cut-off wavenumber k_{cut} . It is based on a model for the inertial and dissipative parts of the spectrum. Without loss of information, it could be used for signals with k_{cut} placed within the inertial or the dissipative range. It was shown that the Pope's model for the dissipative part of the spectrum provides the best fit to the DNS data. As k_{cut} moves towards high-wavenumber part of the spectrum, estimated ϵ_{NCR} deteriorated. As identified, the discrepancies follow from the deviations of the Taylor-to-Liepmann scale λ_n/Λ from unity. It was shown that this ratio could be used as an indicator of the external intermittency. Moreover, an alternative formulation of the second method was proposed, where the variance of velocity derivative is used instead of the number of crossings per length. The rest of the procedure remains the same, that is, the correction factor for the missing part of the spectrum and ϵ are calculated iteratively. Results compare very favourably with the DNS data. This also suggests that in spite of the deviations in the inertial range, the local isotropy assumption is quite well satisfied within the dissipative range. With this study, it was shown that the new methods for TKE dissipation rate retrieval could provide an interesting alternative to the standard approaches.

The second part of the thesis examined the numerical reconstruction of subgrid scales in large eddy simulation using the fractal interpolation technique. For the reconstruction process, values of the stretching parameter d should be specified. This parameter determines the characteristics of the reconstructed signal, which can be derived from its fractal dimension [120]. In previous works, the stretching parameter was chosen to be constant in time and space. To account for its spatial variability, the PDF of the absolute value of the stretching parameter $|d|$ is calculated from DNS data of stratocumulus-top boundary layer, LES data in the same flow configuration and, additionally, measurement data from POST campaign. For this, 1D intersections of velocity field are first low-pass filtered to certain cut-off wavenumbers. Next, an algorithm proposed in Ref. [83] is used to compute the local values of d . It was found that if the cut-off wavenumbers were in the inertial range, the PDFs of the stretching parameter collapsed into one curve, independent of the Reynolds number. I examined the auto-correlation of the stretching parameter in time and observed

that the stretching parameter decorrelates with the characteristic time-scale τ_η and can be chosen randomly after each time step in LES. Next, 1D intersections of filtered velocity field were reconstructed such that d is a random variable with the prescribed, previously determined PDF. Performance of the new approach was compared with FITs with constant values of d . It was shown the energy spectra follow the $-5/3$ scaling more closely and have no spurious modulations if d is random. Moreover, the non-Gaussian, stretched-exponential tails of PDFs of velocity increments are reproduced correctly by the improved model. I investigated these statistics as they quantify internal intermittency of small scale turbulence [52, 70]. The random stretching parameter is also used to construct unresolved scales of POST airborne data (flight 13) and 3-D LES of the stratocumulus-top boundary layer. Statistics of velocity increments showed that the improved fractal sub-grid model is capable of reproducing some of the sub-grid scale features, which might be lost due to finite grid resolution and numerical effects in LES or finite sampling frequency of measurements. In the case of LES field, the fractal reconstruction was extended in 3-D. The divergence-free condition, which can be violated when using FIT, was addressed. It was observed that after two reconstruction steps, the error in mass conservation of the reconstructed field is of the same order of magnitude as the error of filtered LES without reconstruction. Moreover, the computational cost required by FIT was compared with the cost of LES without reconstruction. It was concluded that, even with three reconstruction steps, CPU time of LES with FIT is of the same order of magnitude as the CPU time of LES. Possible applications of the fractal sub-grid model were addressed. I showed that FIT could be used to reconstruct the resolved stresses for a test filter and the residual kinetic energy in LES. It was shown that, based on the preliminary test, the LES velocity field used in the Lagrangian tracking of super-droplet (for the simulation of cloud microphysics) could be improved with FIT.

10.2 Possible outlook

Atmospheric turbulence is complex and can be dominated by multiple dynamics of various scales. For the first part of the thesis, a test on the performance of these methods for TKE dissipation rate retrieval can be performed on a larger experimental dataset or moderate-to-high Re number flow. It will also be interesting to study the performance of these methods in synthetic 2D or 3D turbulent signals.

For the second part of the thesis, this fractal model can be coupled with particle-based methods such as the super-droplet method [14, 125] to predict cloud microphysics in large-eddy simulations of clouds to account for precipitation and motion of aerosols. The fractal model can be improved to account for the anisotropy of atmospheric turbulence and external intermittency.

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