1 Introduction

The turbulent motion of fluids and scalars is a highly complex problem. It is still one of the unsolved problems of classical physics, cf. Nelkin (1992) and Shraiman and Siggia (2000), and the description remains challenging. The understanding of turbulent flows and turbulent mixing is of great interests for many applications. Prominent examples are the turbulent combustion of chemical reactants and the dynamics of the atmosphere or the oceans. In those cases the evolution of the scalar affects the turbulent flow itself. Here, we focus on the case where the scalar is both conserved and passive and does not affect the flow field.

The main difficulties regarding the statistical description of turbulent flows originates from the non-locality and non-linearity of the governing equations. Turbulent flows are characterized by a very great number of degrees of freedom resulting in a wide range of interacting time and length scales. Therefore, a theory for turbulent flows must be a statistical one. Due to the non-locality it is customary to examine turbulent flows by means of two-point statistics. Most understanding of turbulence at high Reynolds numbers is based on the scaling theory developed first by Kolmogorov (1941a,b) and extended later to scalars by Obukhov (1949b) and Corrsin (1951). Based on dimensional arguments, this theory relates the statistics of velocity or scalar increments to the mean energy or scalar dissipation. By the Kolmogorov-Obhukov-Corrsin (KOC) theory the information about the local structure of the turbulent field is lost when taking ensemble averages over fixed separation distances. This issue was overcome by Wang and Peters (2006, 2008) by the theory of dissipation elements. Here, two-point statistics are calculated along gradient trajectories that connect local minimum and local maximum points in the scalar field. The spatial region formed by the ensemble of all gradient trajectories sharing the same extreme points is called dissipation element. They may be parameterized by the linear separation distance and the scalar difference between the extreme points. By this approach the linear separation distance itself becomes an intrinsic stochastic quantity that is determined by the turbulent field. In the present thesis we propose to decompose the signal of a passive scalar along a straight line into piece-wise monotonously increasing or decreasing line segments that start at a local minimum point and end at a local maximum point or vice versa. These line segments can be understood as one-dimensional dissipation elements. Thereby, we retain the property that the decomposition is determined intrinsically by the turbulent field, but because the decomposition is one-dimensional it can be easily related to conventional two-point statistics in the sense of the KOC theory.

At high Reynolds numbers, turbulent flows exhibit strong spatial and temporal fluctuations. The large structures of the flow at an integral length scale depend on the boundary conditions and cannot be considered as universal. On the other hand according to Kolmogorov's similarity hypotheses, cf. Kolmogorov (1941a,b), under the condition of sufficiently high Reynolds numbers, the small-scale structure of turbulent flows is assumed to become statistically isotropic and universal. In this case, it is expected to find generally valid statistics and scaling relations, as proposed by Kolmogorov's 2/3-law. However, small-scale statistics are affected by strong fluctuations of the dissipation; an effect that is called internal intermittency. Thereby, small-scale statistics, that may be described by the probability density function (pdf) of the velocity or scalar increments, depend on scale. At large separation distances this pdf is Gaussian but for separation distances in the inertial subrange it exhibits strong deviations from Gaussianity with progressively longer stretched-exponential tails. The non-Gaussianity becomes even more pronounced toward small scales where the scalar increment can be interpreted as a derivative. The similarity hypotheses propose an universal shape of the pdf of the scalar increment, where a normalization solely by standard deviation accounts for the dependence of the scale. However, the strong fluctuations of the dissipation destroy small-scale universality. This renders the similarity hypotheses invalid for moments larger than the second order. The deviations from the KOC prediction can be further observed by the anomalous scaling of the moments of the structure functions, or alternatively, by the Reynolds number dependence of the higher order non-dimensional moments.

In the course of this thesis we take the classical KOC theory as starting point to examine turbulent mixing of passive scalars. The results of this thesis strongly rely on Direct Numerical Simulations (DNS) that have been conducted for various Reynolds numbers with a Taylor based Reynolds number between 88 and 529. We solve for an incompressible, statistically homogeneous isotropic velocity field, and additionally, we solve for a statistically homogeneous passive scalar with imposed uniform mean gradient. In the course of the first chapter we introduce the governing equations, characteristic numbers and statistical tools. In the second chapter we describe the numerical algorithms, i.e. the pseudo-spectral method and the time stepping schema, of the newly developed highly-accurate flow solver. Then parallelization strategies, code design and code performance are presented. In the third chapter we present characteristic properties of the DNS simulations and conduct a comprehensive validation by means of theoretical results, experiments, and DNS results from other authors. In chapter 4 we derive a generalized evolution equation for the even moments of the scalar increment that accounts for large scale effects. This equation is interpreted as a scalar energy scale-by-scale budget equation. It is first evaluated by means of DNS and later applied in filtered form to *a-priori* and *a-posteriori* studies of Large Eddy Simulations. Additionally, this equation is the starting point to examine the Reynolds number dependence of scalar structure functions in chapter

6. In chapter 5 we introduce the method of turbulent line segments and conduct by means of DNS a statistical analysis of the parameters chosen to describe the line segments. The respective joint pdfs and marginal pdfs are computed and resulting conditional moments are compared with a focus on the Reynolds number dependence. Additionally, the method of turbulent line segments lead to a novel description of the physics behind cliff-ramp structures and provides an estimate for the length scale at which large gradients occur. In chapter 6 we examine the universality of small scales by line segments and conventional statistics, where Kolmogorov's phenomenology is adapted to the method of line segments. Based on conditional statistics we show that an intermediate length scale has a major contribution to the gradient of line segments and that a scale similarity between the moments of mean gradients and the moments of the local gradients exists. We propose a presumed pdf that allows us to compute gradient statistics based on the principle of decomposition and reconstruction of line segments. Furthermore, we adopt the scale-by-scale scalar energy budget equation derived in chapter 4 to show that the non-universality of higher order moments originates from a coupling of dissipative effects to the inertial subrange. Finally, in chapter 7 a brief summary of the main results is given.

1.1 Governing Equations

1.1.1 Velocity Field

We assume that the motion of the fluid is governed by the Navier-Stokes equations and shall restrict ourselves to incompressible and Newtonian fluids. If so, the Navier-Stokes[1] equations read

$$\begin{aligned} \frac{\partial u_j}{\partial t} + u_i \frac{\partial u_j}{\partial x_i} &= -\frac{\partial p}{\partial x_j} + \nu \frac{\partial^2 u_j}{\partial x_i^2} + f_j \,, \quad j = 1,2,3 \\ \frac{\partial u_i}{\partial x_i} &= 0 \,, \end{aligned} \tag{1.1}$$

where p is the pressure, obtained by dividing the dynamic pressure by the density ρ; ν is the kinematic viscosity, and $u_j(\boldsymbol{x}, t)$ the Eulerian velocity field, which depends on position $\boldsymbol{x}$ and time t. f_j denotes an external forcing which acts on large scales only. The Navier-Stokes equations contain all necessary information to fully characterize the motion of turbulent flows. For solving eq. 1.1 adequate initial and boundary conditions must be specified. For simplicity we assume periodic boundary conditions, where all dependent variables fulfill the condition

$$u_i(x_1 + n_1 L, x_2 + n_2 L, x_3 + n_3 L) = u_i(x_1, x_2, x_3) \,, \tag{1.2}$$

[1] The standard rule for summation over repeated indices applies.

for all $\boldsymbol{x}$ and all integers $\boldsymbol{n}$. The period L is taken as 2π. Throughout this work, we further restrict ourselves to statistically isotropic velocity fields. In that case, we do not need to distinguish between mean and fluctuating quantities, and therefore u_j and p denote the velocity and the pressure fluctuations, respectively. The Navier-Stokes equations reveal two important mathematical properties: The non-linearity of the advective term and the non-locality of the pressure term. By taking the divergency of eq. 1.1 and assuming that the forcing term is rotational, we obtain the so called Poisson equation for the pressure

$$\frac{\partial^2 p}{\partial x_i^2} = -\frac{\partial u_i}{\partial x_j}\frac{\partial u_j}{\partial x_i}\,, \tag{1.3}$$

where we have exploited solenoidality of u_j. For periodic domains, the Poisson equation can be inverted by applying a Fourier transform to eq. 1.3. It follows that

$$\widehat{p}_\kappa = \frac{1}{\kappa^2}\mathcal{F}\left(\frac{\partial u_i}{\partial x_j}\frac{\partial u_j}{\partial x_i}\right)\,. \tag{1.4}$$

The forward Fourier transform is denoted by $\mathcal{F}$ and κ is the modulus of the wavevector $\boldsymbol{\kappa}$. The solution of the Poisson equation is defined up to an additive constant, since $\hat{p}_0$ is arbitrary. Equation 1.4 illustrates the non-locality of the pressure field by the application of the Fourier transform.

1.1.2 Scalar Field

Additionally, we consider the motion of a conserved passive scalar $\Phi(\boldsymbol{x}, t)$, governed by the advection-diffusion equation

$$\frac{\partial \Phi}{\partial t} + u_i\frac{\partial \Phi}{\partial x_i} = D\frac{\partial^2 \Phi}{\partial x_i^2}\,, \tag{1.5}$$

where D is the molecular diffusivity. Equation 1.5 is linear in terms of the scalar $\Phi(\boldsymbol{x}, t)$, but $\Phi(\boldsymbol{x}, t)$ is coupled through the convective term in a non-linear way to the velocity field $u_i(\boldsymbol{x}, t)$. The scalar is passive which means that the motion of the scalar has no impact on the velocity field. Furthermore, the scalar is conserved, because eq. 1.5 contains no source or sink term. Examples of scalar turbulence are the temperature field or the motion of a non-reactive contaminant when the concentration is so low that it has no dynamical effect on the flow field.

In order to keep the scalar in a statistically steady state a uniform mean gradient is imposed on the scalar field. To this end the scalar field is decomposed into mean and fluctuating components, i.e.

$$\Phi(\boldsymbol{x}, t) = \Gamma x_2 + \phi(x, t)\,. \tag{1.6}$$

Here, Γ is the magnitude of the uniform mean scalar gradient and $\phi(\boldsymbol{x}, t)$ denotes the fluctuating scalar field. Due to the linearity of eq. 1.5, Γ can be taken as unity without loss of generality. By means of eq. 1.6, we can rewrite eq. 1.5 in terms of the scalar fluctuation

$$\frac{\partial \phi}{\partial t} + u_i \frac{\partial \phi}{\partial x_i} = D \frac{\partial^2 \phi}{\partial x_i^2} - \Gamma u_2 \,. \tag{1.7}$$

1.1.3 Characteristic Numbers

The governing equations can be rewritten in normalized form by introducing a characteristic velocity scale U, a characteristic length scale L and a scalar reference value Φ_{ref}. With $\tilde{x}_i = x_i/L$, $\tilde{u}_i = u_i/U$, $\tilde{t} = tL/U$, $\tilde{p} = p/U^2$ and $\tilde{f}_i = f_i L/U^2$, we obtain for the Navier-Stokes equations

$$\frac{\partial \tilde{u}_j}{\partial \tilde{t}} + \tilde{u}_i \frac{\partial \tilde{u}_j}{\partial \tilde{x}_i} = -\frac{\partial \tilde{p}}{\partial \tilde{x}_j} + \frac{1}{\mathrm{Re}} \frac{\partial^2 \tilde{u}_j}{\partial \tilde{x}_i^2} + \tilde{f}_j \,. \tag{1.8}$$

Only one non-dimensional number, namely the Reynolds number $\mathrm{Re} = UL/\nu$, appears. The scalar transport equation reads in normalized form

$$\frac{\partial \tilde{\Phi}}{\partial \tilde{t}} + \tilde{u}_i \frac{\partial \tilde{\Phi}}{\partial \tilde{x}_i} = \frac{1}{\mathrm{Re}} \frac{1}{\mathrm{Sc}} \frac{\partial^2 \tilde{\Phi}}{\partial \tilde{x}_i^2} \,, \tag{1.9}$$

where the Schmidt number, defined as $\mathrm{Sc} = \nu/D$ appears as additional non-dimensional quantity. The product of Reynolds and Schmidt number is defined as the Peclet number Pe. The Peclet number characterizes the interplay between advection and diffusion effects and can be expressed as

$$\mathrm{Pe} = \mathrm{Re}\,\mathrm{Sc} = \frac{\mathcal{O}(u_i \frac{\partial \phi}{\partial x_i})}{\mathcal{O}(D \frac{\partial^2 \phi}{\partial x_i^2})} \propto \frac{UL}{D} \,. \tag{1.10}$$

1.2 A Statistical Description of Turbulence

Turbulent flows are governed by deterministic equations, cf. eqs. 1.1 and 1.5. But under the condition of high Reynolds numbers, turbulent flows evolve in a complex spatially and temporally stochastic way. The Reynolds number, as the most important non-dimensional number to characterize flows, can be interpreted as the ratio of inertial forces to viscous forces acting on a fluid element. When the Reynolds number is small the viscous forces damp perturbations and the flow remains in a deterministic laminar state. When the Reynolds number exceeds a critical value the flow becomes unstable and a transition from laminar flow to a turbulent flow with strong fluctuations takes place. However, turbulent flows are not fully random and the presence of coherent structures indicate a certain level of organization or

symmetries in a statistically sense. In this section we will introduce the mathematical tools for the statistically description of turbulent flows.

1.2.1 Random Variables

In turbulent flows the variables $u_i(\boldsymbol{x},t)$, $p(\boldsymbol{x},t)$ and $\phi(\boldsymbol{x},t)$ are random variables. A random variable ϕ can be completely characterized by its probability density function $f_\phi(\psi)$, where ψ is the sample-space variable corresponding to ϕ. The mean value of the random variable can be obtained by

$$\langle\phi(\boldsymbol{x},t)\rangle = \int \psi f_\phi(\psi;\boldsymbol{x},t)\mathrm{d}\psi\,, \tag{1.11}$$

and the nth order moment of the random variable is defined by

$$\langle\phi^n(\boldsymbol{x},t)\rangle = \int \psi^n f_\phi(\psi;\boldsymbol{x},t)\mathrm{d}\psi\,. \tag{1.12}$$

The random variable is called centered if the mean of the first moment $\langle\phi\rangle$ equals zero. The centered second moment $\left\langle\phi^2\right\rangle$ is called variance, and the square-root of the variance is called standard deviation and is denoted by σ_ϕ. The dimensionless quantities $S = \left\langle\phi^3\right\rangle / \left\langle\phi^2\right\rangle^{3/2}$ and $F = \left\langle\phi^4\right\rangle / \left\langle\phi^2\right\rangle^2$ are called skewness and flatness, respectively.

The mean value of $\phi(\boldsymbol{x},t)$ can also be obtained directly from a series of numerical or experimental data. In the case of an instationary process the averaging procedure has to be repeated over N realizations

$$\langle\phi(\boldsymbol{x},t)\rangle = \frac{1}{N}\sum_i^N \phi_i(\boldsymbol{x},t) \tag{1.13}$$

and is called ensemble average. For statistically stationary flows the temporal average can be obtained by

$$\langle\phi(\boldsymbol{x})\rangle = \frac{1}{\Delta t}\int_t^{t+\Delta t} \phi(\boldsymbol{x},t')\mathrm{d}t'\,. \tag{1.14}$$

The ergodic theorem states that for a stationary process the temporal and the ensemble average yield the same result. An ergodic variable becomes both uncorrelated and statistically independent with itself for large time differences.

1.2.2 Statistical Symmetries

The Navier-Stokes equations reveal several symmetries. Although generally a single realization of a turbulent field exhibits no obvious symmetries, the averaged quantities reveal statistical symmetries. Turbulent flows are typically described by statistical

methods, like central moments, pdf equations, or two-point correlations. Statistical symmetries can be exploited to simplify these equations and reduce the number of independent variables.

Statistical stationarity[2] holds when the n-point pdf f_n of a random variable $\boldsymbol{u}(\boldsymbol{x}, t)$ is independent of time, i.e.

$$\begin{aligned} &f_n(\boldsymbol{u}_1, \boldsymbol{x}_1, t_1; \cdots ; \boldsymbol{u}_n, \boldsymbol{x}_n, t_n) = \\ &f_n(\boldsymbol{u}_1, \boldsymbol{x}_1, t_1 + \tau; \cdots ; \boldsymbol{u}_n, \boldsymbol{x}_n, t_n + \tau) \,. \end{aligned} \tag{1.15}$$

with an arbitrary time shift τ. Homogeneity correspond to stationarity in space: A n-point pdf of a centered random variable is independent regarding a shift $\boldsymbol{r}$ in space, i.e.

$$\begin{aligned} &f_n(\boldsymbol{u}_1, \boldsymbol{x}_1, t_1; \cdots ; \boldsymbol{u}_n, \boldsymbol{x}_n, t_n) = \\ &f_n(\boldsymbol{u}_1, \boldsymbol{x}_1 + \boldsymbol{r}, t_1; \cdots ; \boldsymbol{u}_n, \boldsymbol{x}_n + \boldsymbol{r}, t_n) \,. \end{aligned} \tag{1.16}$$

As consequence, all central moments are invariant regarding space-translation of their arguments. We restrict ourselves here to centered random variables and allow gradients of mean quantities, but require that gradients of mean quantities are constant. Statistical invariance regarding rotation and reflection is called isotropy

$$\begin{aligned} &f_n(\boldsymbol{u}_1, \cdots , \boldsymbol{u}_n; \boldsymbol{r}_1, \cdots , \boldsymbol{r}_{n-1}) = \\ &f_n(\mathbf{D}\boldsymbol{u}_1, \cdots , \mathbf{D}\boldsymbol{u}_n; \mathbf{D}\boldsymbol{r}_1, \cdots , \mathbf{D}\boldsymbol{r}_{n-1}) \,, \end{aligned} \tag{1.17}$$

where $\mathbf{D}$ is an arbitrary transformation $\mathbf{D} \in \mathrm{O}(3)$, which is the full rotation group. Due to homogeneity and isotropy the mean of a vectorial quantity disappears, i.e. $\langle \boldsymbol{u} \rangle = 0$.

[2] For brevity in the following we will omit the word “statistically”

2 Direct Numerical Simulation of Turbulent Flows

Even for the simplest turbulent flows, an analytical solution of the Navier-Stokes equations is not known. Therefore, a solution of the Navier-Stokes equations can only be obtained by numerical methods. Direct numerical simulation (DNS) solves the Navier-Stokes equations for all scales down to the Kolmogorov length and provides a complete description of the flow, where the three-dimensional flow fields are known as a function of space and time. Because of growing computational capabilities DNS of turbulent flows has become an indispensable tool. cf. Siggia (1981) and She et al. (1990).

In the course of this chapter we present the techniques used to numerically solve the Navier-Stokes equations as well as the evolution equation of a passive scalar. All results presented in this thesis rely on DNS and much effort has been spent to develop an accurate, highly optimized code for the simulation of turbulent flows.

2.1 Pseudo-Spectral Methods

Pseudo-spectral methods are both efficient and accurate, but require a periodic domain, cf. Rogallo (1981) and Canuto et al. (1988). Here, the domain is a cube of size $L = 2\pi$ which is discretized on a grid with N^3 grid points. In real space, the grid is defined as

$$\boldsymbol{x} = (i, j, k)\frac{2\pi}{N}\,, \tag{2.1}$$

where $1 \leq i, j, k \leq N$. The wavenumber components $\boldsymbol{\kappa}$ in Fourier space read

$$\boldsymbol{\kappa} = (i, j, k)\frac{2\pi}{L}\,, \tag{2.2}$$

where $-\frac{N}{2} + 1 \leq i, j, k \leq \frac{N}{2}$. A scalar field ϕ given on the physical grid can now be transformed to Fourier space by

$$\hat{\phi}(\boldsymbol{k}, t) = \frac{1}{N^3}\sum_{\boldsymbol{x}} \phi(\boldsymbol{x}, t)\exp(-i\boldsymbol{\kappa}\cdot\boldsymbol{x}) \tag{2.3}$$

and the Fourier coefficients $\hat{\phi}(\boldsymbol{k}, t)$ can be transformed back to real space by

$$\phi(\boldsymbol{x}, t) = \sum_{\boldsymbol{k}} \hat{\phi}(\boldsymbol{x}, t)\exp(i\boldsymbol{\kappa}\cdot\boldsymbol{x})\,. \tag{2.4}$$

For any real field $\phi(\boldsymbol{x}, t)$ the condition $\hat{\phi}^*(\boldsymbol{\kappa}, t) = \hat{\phi}(-\boldsymbol{\kappa}, t)$ holds, where the star denotes the complex conjugate of $\hat{\phi}(\boldsymbol{\kappa}, t)$. The advantage of this condition is that only one-half of the Fourier coefficients of any real field need to be calculated and stored.

When we evaluate a transport equation in Fourier space, the first derivative of the dependent variable $\phi(\boldsymbol{x})$ can be transformed according to

$$\mathcal{F}\left[\frac{\partial}{\partial x_i}\phi(\boldsymbol{x})\right] = i\kappa_i\hat{\phi}(\boldsymbol{\kappa})\,, \tag{2.5}$$

and the Fourier transform of the second derivative reads

$$\mathcal{F}\left[\frac{\partial^2}{\partial x_i^2}\phi(\boldsymbol{x})\right] = -\kappa_i^2\hat{\phi}(\boldsymbol{\kappa})\,, \tag{2.6}$$

respectively. By using Fourier transform we can thus replace derivative operators by multiplication by the wavenumber. All derivatives appearing in linear terms of the transport equation can be treated in this way. However, the Fourier transformation of a non-linear term in real space

$$\mathcal{F}\left[\phi(\boldsymbol{x})^2\right] = \hat{\phi}(\boldsymbol{\kappa}) * \hat{\phi}(\boldsymbol{\kappa}) \tag{2.7}$$

turns into a convolution in Fourier space. This operation is computationally very expensive and requires $\mathcal{O}(N^{2\cdot 3})$ operations. Therefore, instead of directly evaluating the convolution operation, the multiplication of the non-linear term is computed in real space. This approach requires only $\mathcal{O}(N^3 \log N^3)$ operations and is called pseudo-spectral method since only differentiation is performed in Fourier space.

2.1.1 Velocity Field

We solve the three-dimensional Navier-Stokes equations for incompressible fluids in rotational form

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{\omega} \times \boldsymbol{u} = -\nabla\left(p + \frac{1}{2}\boldsymbol{u}^2\right) + \nu\nabla^2\boldsymbol{u} + \boldsymbol{f} \tag{2.8}$$

with the continuity equation

$$\nabla \cdot \boldsymbol{u} = 0\,, \tag{2.9}$$

where $\boldsymbol{\omega} = \nabla \times \boldsymbol{u}$ is the vorticity, p is the ratio of pressure and density, and ν is the kinematic viscosity. $\boldsymbol{f}$ is a forcing term which acts on large scales only. Equation 2.8 is solved by a pseudo-spectral method in Fourier space. Applying eq. 2.3 to eq. 2.8 yields

$$\frac{\partial \hat{\boldsymbol{u}}}{\partial t} + \mathcal{F}\left(\boldsymbol{\omega} \times \boldsymbol{u}\right) = -i\boldsymbol{\kappa}\hat{P} - \nu\kappa^2\hat{\boldsymbol{u}} + \mathcal{F}(\boldsymbol{f})\,, \tag{2.10}$$