Doctoral Thesis

Entropic Lattice Boltzmann Models for Fluid Dynamics

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ENTROPIC LATTICE BOLTZMANN MODELS FOR FLUID DYNAMICS

A thesis submitted to attain the degree of
DOCTOR OF SCIENCES of ETH ZURICH
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For instance, on the planet Earth, man had always assumed that he was more intelligent than dolphins because he had achieved so much—the wheel, New York, wars and so on—whilst all the dolphins had ever done was muck about in the water having a good time. But conversely, the dolphins had always believed that they were far more intelligent than man—for precisely the same reasons.

Douglas Adams, The Hitchhiker’s Guide to the Galaxy
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Zürich, March 2017

Fabian Bösch
Abstract

The lattice Boltzmann method (LBM) is a modern and highly successful approach to computational fluid dynamics based on a fully discrete kinetic equation and offers an attractive alternative to direct discretizations of the macroscopic continuum equations. However, the original single relaxation-time formulation (LBGK) was plagued by numerical instabilities and prevented the simulation of highly turbulent flows unless prohibitively high resolutions were employed. A number of improvements and variations of LBM attempted to alleviate this issue. In particular, the multiple relaxation-times methods (MRT) take advantage of the additional degrees of freedom in the LBM kinetic system in order to stabilize the solution and improve accuracy. However, the introduction of additional tunable constants must be chosen appropriately depending on the physics and the flow at hand and are not universal, and thus, the problem of stability could not be solved consistently. With the inception of the entropic lattice Boltzmann method (ELBM) which reintroduced the discrete-time equivalent of Boltzmann’s $H$-theorem, the application range has grown widely not only for incompressible turbulent flows, but also for thermal flows, two-phase systems with non-ideal equations of state and has made the simulation of compressible and high Mach number flows possible. The ELBM, however, comes at the price of introducing a fluctuating viscosity.

The main result of this thesis is the development of a new class of entropic MRT models which combine the salient advantages from MRT and ELBM while trying to circumvent their respective disadvantages [1–3]. J. W. Gibbs’ seminal prescription for constructing optimal states by maximizing the entropy under pertinent constraints is used to derive a novel lattice kinetic theory and the the notion of modifying the viscosity to stabilize sub-grid simulations is challenged in this kinetic framework. By exploiting the degrees of freedom of MRT and by compliance to the discrete-time $H$-theorem, the advantages of both MRT and ELBM can be retained and the problems of parameter tuning and fluctuating viscosity can be solved. The resulting models are accurate, adaptive, parameter-free, efficient and, more importantly, very stable.
The entropic MRT models are studied extensively for two- and three- dimensional benchmark simulations at turbulent conditions and compared to experiments, theory and other numerical methods. While the entropic MRT models yield the same results as the LBGK in the resolved limit, and converge towards the Navier-Stokes equations with second-order accuracy, sufficiently accurate results are obtained also at coarse resolutions without the use of sub-grid turbulence models. This made the simulation of high Reynolds number flows with complex boundaries possible which are most relevant for engineering applications.

Due to the general nature of the entropic MRT methods, a number of extensions beyond the incompressible low Mach number regimes were explored and extensions for thermal flows and two-phase flows are presented. Moreover, a novel model for miscible binary mixtures is presented in combination with the entropic MRT collision step. The salient features of this model are the lack of interpolation and the use of thermal multi-speed lattices to account for the different sound speed of the two unequally heavy substances involved. Independent adjustment of the diffusion coefficient and kinematic viscosity of the mixture is assured and the diffusion follows the Stefan-Maxwell model.

To conclude it is shown that entropy maximisation principle can be extended to multiple relaxation-time lattice Boltzmann models to create more stable and computationally efficient LBM models. This principle of entropy maximization is applied without nominal modification of viscosity and is extended to not only high Reynolds number flows but also thermal, mixture and multi-phase flows. This principle is also shown to be lattice independent and generic nature thus opening a possibility of new class of LB models that are more robust to under-resolution and have a wide range of applications.
Zusammenfassung


Die entropischen MRT Methoden lassen sich dank ihrer allgemeinen Form auf eine Reihe von Erweiterungen jenseits der inkompressiblen Strömungen anwenden und Beispiele von thermalen und Zwei-Phasen Strömungen werden gezeigt.


# Contents

Abstract v

Zusammenfassung vii

1 Introduction 1

1.1 Motivation .............................................................. 2

1.2 Outline of the Thesis .................................................. 3

2 Lattice Boltzmann Method 7

2.1 Lattice Gas Automata .................................................... 8

2.2 Lattice Bhatnagar-Gross-Krook Model ................................ 10

2.3 Moments and Multiple Relaxation Time Models ................... 14

2.4 Moments for standard Lattices ....................................... 21

2.4.1 Moment Representation for D2Q9 .............................. 21

2.4.2 Moment Representation for D3Q27 .............................. 23

3 Exact Lattice Boltzmann 25

3.1 Kinetic Equation .......................................................... 26

3.2 Exact Integration .......................................................... 27

3.3 Discussion ................................................................. 30

3.4 Conclusions ............................................................... 31

4 Entropic Lattice Boltzmann Method 33

4.1 Entropic Equilibrium .................................................... 33

4.2 Isentropic Condition ..................................................... 36

4.3 Results and Discussion ................................................ 36

4.4 Conclusions ............................................................... 42

5 Entropic Multi-Relaxation Models 45

5.1 Moment Grouping ......................................................... 46

5.2 Realization in Two and Three Dimensions ....................... 48
5.3 Discussion ......................................................... 49
5.4 Implementation .................................................. 52
5.5 Hydrodynamic Limit of KBC Models ......................... 53
5.6 Generalization .................................................... 56
5.7 Boundary Conditions ............................................ 57
  5.7.1 Domain Boundary Conditions .......................... 57
  5.7.2 Wall Boundary Conditions ............................... 58

6 Convergence and Accuracy in the Resolved Limit 61
  6.1 Green-Taylor Vortex Flow ................................. 61
  6.2 Periodic Double Shear-Layer ............................... 63
  6.3 Conclusions ................................................... 67

7 Decaying Homogeneous Isotropic Turbulence 69
  7.1 Two-Dimensional Turbulence ............................... 71
  7.2 Kida-Vortex Flow ............................................. 79
    7.2.1 One-Point Statistics .................................. 82
    7.2.2 Two-Point Statistics .................................. 86
    7.2.3 Stabilizer $\gamma$ and the LBGK Limit ................ 87
    7.2.4 Convergence to the Navier-Stokes Equations at Small Scales 87
  7.3 Large Reynolds Numbers .................................... 91
  7.4 Conclusions .................................................. 92

8 Complex and Wall-bounded turbulent Flows 95
  8.1 Turbulent Channel Flow .................................... 95
  8.2 Turbulent Pipe Flow ....................................... 99
  8.3 Flow around circular Cylinder ............................ 102
  8.4 Flow around a reference Car Model ....................... 104
  8.5 Further Applications ...................................... 107
    8.5.1 Flow past Sphere ..................................... 107
    8.5.2 Flow in Engine-like Geometry ....................... 107
    8.5.3 Transitional Flows past Airfoil ..................... 110
  8.6 Conclusions ................................................ 112

9 Extensions ..................................................... 113
  9.1 Thermal Flows .............................................. 113
  9.2 Two-Phase Flows .......................................... 117
  9.3 Binary Mixtures ............................................ 122
Chapter 1

Introduction

Fluid dynamics and its manifestations impact our lives in numerous aspects, from predicting next week’s weather to drug delivery through the cardiovascular system, or industrial applications such as an automotive engine, and thus, predicting the behaviour of fluids is of profound importance.

However, the theoretical study of fluid dynamics is complex and remains challenging. The fundamental basis of the continuum description is provided by the Navier-Stokes equations, for which only few analytical solutions are known for simplistic situations.

The most interesting phenomena arise when the dissipative forces are small compared to the inertial forces, characterized by a large Reynolds number, and the flow becomes turbulent such that the motion of the fluid appears chaotic and unpredictable and eludes a comprehensive analytical description. The range of time and length scales in these situations is immense and causes troubles for both experimental investigations as well as for numerical approaches.

With the rapid increase in computing power, numerical simulations of fluid flows have become an important tool for predictive purposes, as well as to gain in-depth insight into the fundamental phenomena arising in fluid mechanics.

However, the computational demand of direct numerical simulations (DNS) of the Navier-Stokes equations, which account for all scales in the flow, is large and becomes quickly prohibitive, even for the largest supercomputers.

Hence, attempts to reduce the computational expenses are numerous; often the equations are filtered (averaged) and the unresolved scales are modelled. Such turbulence models include eddy-viscosity models, Reynolds-stress models, large eddy simulations (LES) and probability density function (PDF) methods [4]. While much faster, these simplified models bear the inevitable loss of generality compared to the direct approach and careful selection of appropriate parameters and models depending on the flow and geometry.
are typically required. Thus development of efficient, high-fidelity, robust and accurate solvers which are general enough to cope with any turbulent flow, irrespective of its complexity and domain characteristics, is a topic of tremendous interest.

1.1 Motivation

The lattice Boltzmann (LB) method [5, 6] is a modern and highly efficient approach based on kinetic-theory to computational fluid dynamics and computational physics of complex flows and fluids, with applications ranging from turbulence [7] to flows at a micron scale [8] and multiphase flows [9, 10], to relativistic hydrodynamics [11], soft-glassy systems [12] and beyond. The LB method solves numerically a fully discrete kinetic equation for populations $f_i(x, t)$, designed to reproduce the Navier-Stokes equations in the hydrodynamic limit. Populations correspond to discrete velocities $v_i, i = 1,\ldots, q$, which fit into a regular spatial lattice with the nodes $x$.

The macroscopic behaviour of the target equation is realized as the limiting behavior of the underlying discrete dynamics of the populations. In contrast to molecular dynamics (MD) and other kinetic methods based on the Boltzmann equation, the LB particles follow deterministic and simple collision rules, much alike the lattice Gas (LG) automata. The mesoscopic LB method offers a number of attractive features. In particular, the particles or populations $f_i$ are advected along the lattice links in a discrete and exact manner and thus the process of convection is loss-free and does not result in artificial numerical dissipation. While the advection is linear, the non-linearity in LB is exposed only locally in the evaluation of the local equilibrium. Moreover, the pressure is available explicitly through the ideal gas equation of state and is thus local as well. This is in sharp contrast to conventional computational fluid dynamics (CFD) methods for incompressible flows which attempt to discretize the Navier-Stokes equations directly. The quadratic advection term in the Navier-stokes equations results in a non-local and non-linear momentum transport and the pressure is only available through the solution of the global pressure-Poisson equation in the strictly incompressible case.

Moreover, due to this locality, the LB is particularly well suited for a straightforward parallelization for a distributed memory architecture. With its simplicity and operational efficiency LB is a natural choice for high performance computing (HPC).
Despite its promising nature the LB in its original form has suffered from teething troubles. In particular, the simulation of high Reynolds number flows was only possible using a large grid resolutions comparable to DNS simulations. In order to improve the numerical stability for under-resolved simulations a number of attempts have been proposed, such as the popular multiple-relaxation time models (MRT) [7, 13–17], and other models with non-linear collisions [18]. The MRT models, in particular, expose additional degrees of freedom which may be used to remedy the problem of instability. However, flow dependent parameter tuning may be necessary and high Reynolds numbers are still not universally achieved [19].

An adequate solution came about with the inception of the entropic lattice Boltzmann method (ELBM) [20–24] which restored the second law of thermodynamics (Boltzmann's $H$-theorem for the discrete LB method). With ELBM turbulence simulations [25–27] at large Reynolds numbers became possible. The ELBM is also used to simulate multi-phase flows [10, 28], thermal flows [29, 30] and compressible and super-sonic flows [31–33]. However, the ELBM introduces an adaptive relaxation time which results in a fluctuating effective viscosity which can be viewed as an implicit sub-grid model [24]. This begs the question whether a LB model can be constructed which retains a fixed nominal viscosity as in the standard LB but achieves similar numerical stability as ELBM.

In this thesis, a combination of the pertinent ideas of MRT and ELBM is described which results in a new type of LB models [1–3]. By exploiting the degrees of freedom of MRT and by approximate compliance to the $H$–theorem, the advantages of both methods can be retained and the problems of parameter tuning and fluctuating viscosity can be solved. The resulting family of entropic MRT models, are accurate, adaptive, parameter-free, efficient and also supremely stable and may provide the long sought-after unification of the scattered field of different multi-relaxation models. In the remainder of this thesis, we shall use the acronym KBC for these models, which was derived from the list of authors in the first publication [1].

1.2 Outline of the Thesis

- Chapter 2: The lattice Boltzmann method is introduced from a historical perspective, as a successor of the earlier Lattice Gas automata and the basic lattice Bhatnagar-Gross-Krook model (LBGK) is described in detail.
The lattice Boltzmann equation is recast in an equivalent system of moment equations. The basics behind the multiple relaxation time models (MRT) are explained and explicit moment representations for the standard lattices are given.

- Chapter 3: The connection between the discrete lattice Boltzmann equation and the continuous-time-space kinetic theory is investigated. Details about the common discretization procedure are given and the difference between the exact integration are pointed out.

- Chapter 4: The entropic lattice Boltzmann method (ELBM) is presented along with the discrete version of the $H$-theorem. Implications of the entropic step are discussed and results from a turbulent flow simulation are used to illustrate the inner workings of the built-in sub-grid model.

- Chapter 5: The main result of the thesis is presented: the development of the KBC models as a combination of the multiple relaxation time idea and the entropic lattice Boltzmann method. A detailed derivation of the hydrodynamic limit is presented. Details on the implementation and realization in two and three dimensions are given along with a description of appropriate boundary conditions.

- Chapter 6: The KBC models are applied to simple two-dimensional flow to assess accuracy, stability and sensitivity to small perturbations. Comparisons are drawn with respect to the entropic lattice Boltzmann method and the standard lattice Boltzmann method.

- Chapter 7: The KBC models are used to simulate homogeneous isotropic turbulence in two and three dimensions. Various statistical quantities are measured and compared to theory. The stability and performance of the KBC models with respect to the entropic and standard lattice Boltzmann method is assessed.

- Chapter 8: The KBC models are applied to complex wall bounded turbulent flows relevant for engineering applications. The accuracy of the results is discussed in the light of under-resolved simulations and comparisons with theory and experiments are given.

- Chapter 9: Some extensions of the KBC models which incorporate more physics are discussed. In particular, models for thermal flows and two-
phase flows are armed with the KBC stabilization and simulation results are presented. A new model for the simulation of binary miscible mixtures is presented which is based on a larger multi-speed lattice. The KBC methodology is applied on top and results are presented and compared to theory.
Chapter 2

Lattice Boltzmann Method

Perhaps from the beginning of the sixties of the last century the increasing power of (super-) computers has started opening the field of computational physics in general and of computational fluid dynamics (CFD), in particular. It has been understood early that especially for the investigation of complex non-linear phenomena analytical approaches may not be able to answer all fundamental questions of physics. Take turbulence as an example: since the seminal works of Kolmogorov and Batchelor new insights have been sparse, except perhaps for the corrections due to the intermittent behaviour of flows at large but finite Reynolds numbers. It is therefore just but natural to look for answers to carefully designed and controlled in silicio experiments. The variety of methods to do so is vast, though. When we look at the problem of non-equilibrium continuum hydrodynamics we can identify quite different approaches.

At a molecular level one can, in principle, study this problem through methods from statistical mechanics such as Molecular Dynamics (MD). The sheer amount of molecules and their relative interactions, though, required to come close to a state which can be viewed as continuum is enormous. Still today, simulations at this level would require an immense amount of computational resources if feasible at all.

At the kinetic level, Ludwig Boltzmann's equation for the evolution of one-particle distribution functions with binary collisions serves as starting point for the understanding of a moderately rarefied gas [see 34–36, for a detailed discussion and derivation]. Solving this equation directly (numerically) poses a rather involved challenge, however, due to the complicated particle-particle interactions (collision integral). Statistical methods like Discrete Simulation Monte Carlo and Discrete Velocity models [see cfg. 37, 38] are preferentially used. The efficiency of such methods is however rather poor in the continuum
limit. Moreover, it is still today unclear whether the Boltzmann equation converges to the Navier-Stokes-Fourier equations in general. The continuum approximations (Navier-Stokes-Fourier equations) which are directly implied by macroscopic mass, momentum and energy conservation, on the other hand, have been and still are the model of choice by many for the task of simulating fluid dynamics problems and studying hydrodynamics. Direct numerical simulations (DNS) thereof provide accurate and reliable results in the small Knudsen number regime where the continuum assumption holds. The cost of such an approach is high, though. Not only are the computational resources needed to study a fully resolved flow prohibitively high for large enough Reynolds numbers, but also the methods itself are complicated and require careful treatment of boundary conditions, for example. Thus, DNS has been restricted to relatively simple flows with a limited range in Reynolds numbers. In order to alleviate this drawback, the equations are often filtered (averaged) and the sub-grid scales (unresolved scales) are modelled. Such turbulence models include eddy-viscosity models, Reynolds-stress models, large eddy simulations (LES) and probability density function (PDF) methods [4]. By incorporating a model one inevitably loses the generality of the direct approach and careful selection of appropriate parameters and models depending on the flow and geometry are required.

2.1 Lattice Gas Automata

A quite different approach to understand and simulate non-equilibrium hydrodynamics emerged in the late seventies and early eighties. The preconditions were simple: building a kinetic system which is simple and efficient and reproduces the large scale behaviour (the incompressible Navier-Stokes equations, in particular).

Based on the Cellular Automaton, introduced by John von Neumann (1966) and Stanislaw Ulam, the theory of lattice gas (LG) emerged. In essence the lattice gas automaton consist of a space filling lattice where each lattice link can be populated by one particle only or can be left unpopulated. These "boolean particles" can only travel along their lattice link to the next node (streaming step), and thus space and time are fully discretized in this microworld. Once arrived at a node a set of collision rules redistributes the particles to different lattice directions. These rules must ensure local mass and linear momentum conservation. Averaging (in space and/or time) of the bit populations yields
distribution functions from which macroscopic variables such as density and momentum can be computed by integration over the velocity space. A sufficiently symmetric lattice with appropriate collisions can be shown to converge to the incompressible Navier-Stokes in the low Mach number limit, albeit with spurious defects.

The first fully deterministic LG kinetic system was proposed by Hardy et al. [40] (HPP). The underlying square two-dimensional lattice, however, lacks Galilean invariance, isotropy and the viscosity shows a scale dependence (in 2D) [see also 41]. Some of the drawbacks of this early attempt were overcome by the models of Frisch et al. [41] and d'Humieres et al. [42] which use probabilistic collision rules and are based on the FHP (hexagonal) lattice in 2D and the FCHC (pseudo-four-dimensional, face-centered-hypercubic) lattice in 3D. The collision rules imply a Fermi-Dirac local equilibrium distribution, dependent only on the locally conserved quantities. This, however, results in a spurious velocity dependence of the pressure and a density dependent non-linear advection term (non-Galilean invariance). Arguably, at low Mach numbers, when the fluctuations of the density are small, this kinetic system can still be a valid tool for the simulation of hydrodynamics, but does not reduce to the Navier-Stokes equation in general [43].

The lattice gas has many attractive properties, nonetheless. It provides intrinsic numerical stability by supporting an H-theorem analogous to the Boltzmann equation where the equilibrium states are found as a minimum of the H-function. It is simple and efficient and inherently parallel, due to its locality, and can thus be simulated without difficulties on large distributed memory machines. Another important advantage is the relative simple treatment of boundary conditions which can be handled in the microscopic perspective where particles get (specularly) reflected at solid walls. As stated earlier, obvious drawbacks are the spurious terms in the macroscopic equation. Not last, the LG is known for a bad signal to noise ratio. This requires (spatial and/or temporal) averaging over large areas and long times and reduce its computational efficiency.

Frisch et al. [44] realized that instead of working with boolean particles one can directly write (and simulate) an evolution equation for the distribution functions. This implies a change from the boolean world to real variables and eliminates the problem of noise in the simulation altogether. This equation was derived under the assumption of molecular chaos (particles entering the collision do not have correlation) analogous to the Boltzmann equation. And
indeed, when expanding the kinetic equation to first order the discrete velocity continuous space-time Boltzmann equation,

\[ \partial_t f_i + v_i \partial_{v_i} f_i = \Omega(f), \]

(2.1)
is recovered with \( f_i \) being the mean populations (or distribution functions), and the particle velocity \( v_i \) and the collision operator \( \Omega \). The underlying kinetic equation was subsequently termed "Lattice Boltzmann equation" (LB equation).

### 2.2 Lattice Bhatnagar-Gross-Krook Model

McNamara et al. [45] carried out first simulations of the LB equation using the full Lattice Gas collision rules in an attempt to measure the viscosity. Shortly after that Higuera et al. [46], based on the previous work of Frisch et al. [41], quantitatively investigated the novel Lattice Boltzmann equation derived from the Boltzmann assumption. However, it was found that the collision operator can be simplified further by linearizing around the zero velocity equilibrium, assuming the double limit of small Mach number and Knudsen number. They concluded, that the LB model, while free from noisy fluctuations, offers the same advantages than LG, that is to say inherent parallelism, simplicity and ease of boundary treatment.

The collision operator was thereafter made independent from the underlying boolean microdynamics (LG collision rules) by allowing so-called enhanced collisions [13]. This new class of LB used a real collision matrix, which was essentially dictated by symmetry arguments (dependence on the angles of the microscopic velocities only) and the usual local conservation of mass and momentum. This lead to a more general and more efficient LB scheme, albeit with the same Fermi-Dirac equilibrium as the LG models and thus suffering from the same drawbacks (non-Galilean invariance, velocity dependent pressure).

One crucial difference to the LG, however, was pointed out by Benzi et al. [5]: while the Lattice Gas comes with an H-theorem, the LB with enhanced collisions does not. They analyzed the stability of this method and while linear stability can be achieved by a proper choice of the collision matrix, non-linear flows may evoke numerical instabilities with potentially catastrophic consequences. The cause of these instabilities was mainly attributed to non-positive populations which are not a-priory impossible as in the LG.
It was noted, that the dynamics of higher order moments of the LB model could also be suppressed by reconstructing them every time from the lower order hydrodynamic moments, possibly to the advantage of numerical stability. This approach was later further investigated in the so-called regularized LB schemes [16, 47]. Nevertheless, simulations of two-dimensional flows around cylinders and two-dimensional turbulence at low Reynolds numbers, as well as three-dimensional flows through porous media were already possible. The authors also pointed out the dual viewpoint on the Lattice Boltzmann equation: on the one hand, first order expansion of the discrete LB equation, originating from the LG, leads to the discrete velocity Boltzmann equation, but a particular finite difference approximation of the latter will result in the LB equation, in turn. We will expand on this subject and its subtleties further in Chapter 3.

Almost at the same time, Chen et al. [43] and Qian et al. [48], proposed what we still consider today as the basic LB equation. The collision matrix introduced in Higuera et al. [13] was further simplified to be of diagonal form and with each element identical which effectively leads to a single relaxation time model similar to the famous BGK approximation to the Boltzmann equation [49]. Therefore, this model is also called lattice BGK model (LBGK). More importantly, the local equilibrium was no longer following a Fermi-Dirac distribution but was rather derived from the local Maxwellian (Maxwell-Boltzmann distribution). In consequence, Galilean invariance could be established in the non-linear advection term, and by using a rest particle, with zero microscopic velocity, the spurious dependence of the pressure on the square of velocity could be eliminated. Thus, the LBGK model correctly recovers the Navier-Stokes equation in the hydrodynamic limit with a fixed lattice dependent speed of sound. The only free parameter in this model is used to set the kinematic shear (and bulk) viscosity. Qian et al. [48], unlike previous works, proposed a list of square lattices with varying number of velocities introducing the \( DdQq \) nomenclature, with the dimension \( d \) and number of populations (or velocities) \( q \).

The fully discrete lattice Boltzmann equation reads

\[
f_i(x + \Delta t v_i, t + \Delta t) = f'_i \equiv (1 - \beta) f_i(x, t) + \beta f^{\text{mirr}}_i(x, t). \tag{2.2}
\]

Here the left-hand side is the propagation of the populations along the lattice links (space-time independent microscopic velocity vectors \( v_{i\alpha} \)), while the
right-hand side is the so-called post-collision state \( f' \) and the parameter

\[ \beta \in [0, 1] \]  \hspace{1cm} (2.3)

determines the rate of relaxation. Different LB models are discriminated by the choice of the mirror state \( f_i^{\text{mirr}} \) [50]. The famous lattice Bhatnagar-Gross-Krook (LBGK) model [43, 48], which made realization of hydrodynamics possible in the first place, can be recovered by the choice

\[ f_i^{\text{mirr}} = 2f_i^{\text{eq}} - f_i. \]  \hspace{1cm} (2.4)

The local equilibrium population \( f_i^{\text{eq}} \) depends on space and time only due to locally conserved quantities. Here, \( f_i^{\text{eq}}(\mathbf{x}, t) = f_i^{\text{eq}}(\rho(\mathbf{x}, t), j_\alpha(\mathbf{x}, t)) \) where

\[ \rho \equiv \sum_i f_i \equiv \sum_i f_i^{\text{eq}} \]  \hspace{1cm} (2.5)
\[ j_\alpha \equiv \rho u_\alpha \equiv \sum_i f_i v_{i\alpha} \equiv \sum_i f_i^{\text{eq}} v_{i\alpha}. \]  \hspace{1cm} (2.6)

In other words, the zeroth and first order moments of populations \( f_i \) are locally conserved (remain unchanged by the collision) and yield the macroscopic density and momentum.

In the lattice Boltzmann method, the time step \( \Delta t \) and the lattice spacing \( \Delta x \) are connected by the relation \( \Delta x = \Delta t v_\parallel \), where \( v_\parallel \) denotes a discrete velocity vector along the Cartesian axis. By choosing \( \Delta t = 1 \) and integer-valued discrete velocities, the lattice nodes have integer-valued spatial coordinates. Figure 2.1 illustrates the advection step on a lattice in two dimensions with nine populations (\( D2Q9 \) lattice).

The process of collision (right hand side of Eq. (2.2) with definition (2.4)) is local in space and time and brings the populations towards the local equilibrium and further. This \textit{over-relaxation} property illustrates also a major difference between the continuous Boltzmann BGK model and the discrete system at hand and is eventually the reason for the ability of the LB method to achieve low viscosities (see also Chapter 3).

The target equations are the (weakly compressible) isothermal Navier-Stokes equations,

\[ \partial_t \rho + \partial_\alpha (\rho u_\alpha) = 0, \]  \hspace{1cm} (2.7)
\[ \partial_t (\rho u_\alpha) + \partial_\beta (\rho u_\alpha u_\beta) = -\partial_\alpha p + \partial_\beta \left[ \nu \rho \left( \partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{D} \partial_\gamma u_\gamma \right) \right] \]  \hspace{1cm} (2.8)
\[ + \frac{2}{D} \partial_\beta \left[ \zeta \rho \partial_\gamma u_\gamma \right], \]
with the pressure following the ideal gas law at fixed temperature,

\[ p = \rho c_s^2, \]  

the (finite) speed of sound \( c_s \), kinematic shear and bulk viscosity \( \nu \) and \( \zeta \), respectively. In order for the discrete kinetic system (2.2) to recover the target equations in the low Mach number and hydrodynamic limit certain properties must be met by the local equilibrium. In particular, the second and third-order equilibrium moments must yield the corresponding Maxwell-Boltzmann moments (neglecting higher order velocity terms due to the low Mach number assumption),

\[ P_{\alpha \beta}^{eq} = \sum_i f_i^{eq} v_i \delta_{\alpha \beta} + \rho u_\alpha u_\beta, \]  
\[ Q_{\alpha \beta \gamma}^{eq} = \sum_i f_i^{eq} v_i \delta_{\alpha \beta \gamma} + \rho u_\alpha \delta_{\beta \gamma} + \rho u_\beta \delta_{\alpha \gamma} + \rho u_\gamma \delta_{\alpha \beta} + O(u^3). \]

The finite number of discrete velocities, however, implies a closure relation on the moments, and for the low symmetry (standard) lattices (such as \( D2Q9 \),...
D3Q15, D3Q19 and D3Q27) we have that $v^3_{ia} \equiv v_{ia}$, see Table 2.1 for a list of the discrete velocities and according weights. As a consequence, the speed of sound $c_s$ cannot be chosen arbitrarily but is fixed,

$$c_s = \frac{1}{\sqrt{3}}.$$ (2.12)

As mentioned earlier, a suitable local equilibrium was found as a discretization of the local Maxwellian (through a Gauss-Hermite quadrature) and truncated to second order in velocity,

$$f_{i}^{\text{eq}} = W_i \rho \left[ 1 + \frac{v_{i\alpha} u_\alpha}{c_s^2} + \left( \frac{v_{i\alpha} v_{i\beta} - c_s^2 \delta_{\alpha\beta}}{2c_s^4} \right) u_\alpha u_\beta \right].$$ (2.13)

The weights $W_i$ appearing in the local equilibrium are lattice dependent and dictated by isotropy of the even-order higher velocity tensors (here fourth order). For a different derivation of the equilibrium consistent with the discrete H-theorem see Section 4.1.

With these ingredients the Lattice Boltzmann BGK model recovers the incompressible Navier-Stokes equation with kinematic shear (and bulk) viscosity

$$\nu = \zeta = c_s^2 \Delta t \left( \frac{1}{2\beta} - \frac{1}{2} \right).$$ (2.14)

For a formal derivation of the hydrodynamic limit the reader is referred to Section 5.5.

### 2.3 Moments and Multiple Relaxation Time Models

Almost immediately after its inception, the LBGK model has taken lead in the lattice Boltzmann approach to the simulation of incompressible flows [5, 43, 48, 51] and complex hydrodynamic phenomena [6, 52], and remains the “working horse” of the LB methods to-date. Popularity of LBGK is primarily based on its simplicity and exceptional computational efficiency. It is unfortunate, and was soon realized, that LBGK shows severe deficiencies (disruptive numerical instability) already at relatively low Reynolds numbers unless a rather high resolution is employed, which quickly becomes computationally prohibitive. This precluded the LB method to make a sustainable impact in the field of computational fluid dynamics.
A number of approaches can be found in the literature intended to alleviate this issue. In particular, the popular multiple relaxation-time (MRT) models are promising candidates for a remedy. In the following paragraphs, we summarize the basic ideas behind the MRT models which also serve as starting point for the development of the entropic variant thereof (the KBC models). The \( q \)-dimensional kinetic space spanned by the populations can be represented by any linear combination of \( f_i \) equivalently. One class of such alternative basis are called (velocity-) moments due to their resemblance to statistical moments. Examples thereof were already introduced through the locally conserved quantities (the macroscopic variables) in Eqs. (2.5), (2.6) and equilibrium higher order moments (2.10), (2.11). In general we define the class of natural moments as \( \rho M_{pqr} \), where locally conserved density \( \rho \) is factored out for simplicity,

\[
\rho M_{pqr} = \left\langle f_i v_{ix}^p v_{iy}^q v_{iz}^r \right\rangle, \quad p, q, r \in \mathbb{N}_0,
\]  

(2.15)

and the angular brackets denote summation over the velocity index \( i \). Equation (2.15) is written for the three-dimensional case but is trivially transformed to two dimensions by dropping the last factor associated with the \( z \) component of the velocity vector. The moment representation is particularly convenient for the lower order moments can be interpreted as physical quantities. Another popular basis is given by the central moments of the form

\[
\rho \tilde{M}_{pqr} = \left\langle f_i (v_{ix} - u_x)^p (v_{iy} - u_y)^q (v_{iz} - u_z)^r \right\rangle, \quad p, q, r \in \mathbb{N}_0,
\]  

(2.16)
where the peculiar vectors are centred around local velocity.
In general, the coefficients in representations (2.15) and (2.16) can be assembled in a matrix $\Theta$ and thus the vector $f$ of populations can be related to the vector of moments $m$ through a linear map,

$$\Theta f = \rho m,$$

(2.17)

where $\Theta \in \mathbb{R}^{q \times q}$ is quadratic and invertible. Some other popular linear basis representations adopt orthogonal basis functions with respect to the standard scalar product or a weighted scalar product.

On the other hand, each population can now be expressed as function of the moments by inverting the matrix $\Theta$,

$$f = \rho \Theta^{-1} m.$$

(2.18)

Thus, each population can be represented by a linear combination of the non-conserved moments. The density $\rho$ and velocity $u$ (conserved moments) appear linearly in case of the natural moment basis, while the populations in the central moment basis are polynomial functions thereof.

By applying the transform $\Theta$ to the LB system (2.2), we can write the individual relaxations for the moments $m_i$,

$$m'_i = (1 - \beta) m_i + \beta m_i^{\text{mir}},$$

(2.19)

where $m'_i$ denotes the post-collision state of moment $m_i$ and their mirror states are given by

$$m_i^{\text{mir}} = \gamma_i m_i^{\text{eq}} + (1 - \gamma_i) m_i,$$

(2.20)

where the moment $m_i^{\text{eq}}$ is evaluated at the local equilibrium. Thus, we can, conceptually, apply the relaxation (collision) in the moment space and reconstruct the post-collision populations $f'_i$ from relation (2.18) (using the updated moments (2.19)) which are then advected in the usual LB streaming step. When we set parameters $\gamma_i = 2$ the LBGK model is recovered. It is important to note that the macroscopic equations are recovered by a projection of the kinetic system onto the lower order moments $\rho, u_x, u_y$. The dimension $q$ of the kinetic space populated by $f_i$ is usually greater than strictly necessary for recovering the Navier-Stokes equations. In three dimensions, for instance, ten linearly independent basis vectors would suffice to represent the conserved variables and the symmetric stress tensor (2.10). The higher order moments are thus in our hands, in principle, and they play an important role for the
numerical stability of the scheme. Thus, we may choose a value different from the usual LBGK choice \( \gamma_i \neq 2 \) for these moments. Although it can be shown that the coupling to the non-hydrodynamic higher moments ("ghosts") cannot be chosen arbitrarily in the limit \( \text{Ma} \to 0 \) \cite{53}, independent relaxation of these moments may have favourable effects on the numerical scheme’s stability and accuracy. Precisely this observation has been widely used to construct models with the goal to stabilize the LB scheme, among which are the MRT and KBC models.

The choice of \( \gamma_i \) is constrained by symmetry properties, however, and has to lead to the correct macroscopic limit. Using the Chapman-Enskog method it can be shown that the hydrodynamic limit is not affected to the pertinent accuracy of the model when changing the relaxation of moments of order 3 and higher (see also Section 5.5) for the incompressible flows.

The MRT class of LB models separate the relaxation into various groups based on separation of scales between the fast and slow varying moments and can be used to construct more stable LB schemes. Following this line of thinking, several MRT schemes were suggested for the choice of relaxation of higher order moments (beyond the pressure tensor) \cite{13–15}. They differ in the number of independent relaxation parameters, their respective values, and the moment representation used as basis for spanning the kinetic space. Let us give a short overview of the most popular MRT models.

**Original MRT LB Model** The original MRT model \cite{14, 17, 54} starts from the natural moment representation (2.15). Upon orthogonalization of the matrix \( \hat{M} = \rho \Theta^{-1} \) with the Gram-Schmidt procedure one ends up in

\[
\hat{m} = \hat{M} f, \tag{2.21}
\]

with orthogonal matrix \( \hat{M} \) and a different set of moments \( \hat{m} \), see also \cite{55}. Note that with this procedure the kinematic (conserved) moments remain identical to their natural moment counter-part because they are already orthogonal to each other in the sense of the standard scalar product. The mirror state moments are then defined by

\[
\hat{m}_i^{\text{mirr}} = \gamma_i \hat{m}_i^{\text{eq}} + (1 - \gamma_i) \hat{m}_i, \tag{2.22}
\]

and the parameters \( \gamma_i \) correspond now to the relaxation with respect to the moments \( \hat{m}_i \), and are subsequently chosen based on a linear analysis of the linearized hydrodynamic equations \cite{17}, but for a specific viscosity only. The
set of fixed parameters attained in this way for the D3Q19 lattice was also used by [56] for periodic turbulent flow simulations, where they reported reliable results. In [19], the same model was tested and found reliable and stable for the lid-driven cavity flow. However, it produced spurious artifacts for the turbulent channel flow at $Re_τ = 200$. These oscillations in the bulk of the flow resulted in a decay of the solution with time and persisted also after an increase of resolution. In contrast, the same simulation run with LBGK returned the expected results. It may be argued whether the relaxation constants from [17] are appropriate for all flows. Results from [19] indicate otherwise. This is also confirmed by [18] who state that MRT can be both more accurate and stable than LBGK or less so, depending on the choice of the relaxation parameters.

**Two-relaxation-time LB Model** The two relaxation time lattice Boltzmann model (TRT) was first introduced to extend the LB to advection and anisotropic-dispersion equations [57] and subsequently also used for hydrodynamics [58, 59]. The primary moments here are defined as

$$\hat{m}_i = (f_i + f_{-i})/2, \ i \ even, \quad (2.23)$$

$$\hat{m}_i = (f_i - f_{-i})/2, \ i \ odd, \quad (2.24)$$

with $f_{-i}$ being $f_i$’s opposite-pointing population and the two relaxation constants are associated with the even and odd moments, respectively,

$$\hat{m}_i^{\text{mirr}} = γ_e \hat{m}_i^{\text{eq}} + (1 - γ_e) \hat{m}_i, \ i \ even, \quad (2.26)$$

$$\hat{m}_i^{\text{mirr}} = γ_o \hat{m}_i^{\text{eq}} + (1 - γ_o) \hat{m}_i, \ i \ odd, \quad (2.27)$$

with $γ_e = 2$ in order to recover the correct hydrodynamic equation with kinematic viscosity (2.14). Equivalently, the mirror state in (2.2) can be written here as

$$f_i^{\text{mirr}} = γ_0 f_i + (1 - γ) f_i^{\text{eq}} - (1 + γ) (f_{-i} - f_{-i}^{\text{eq}}), \quad (2.28)$$

with $γ = λ_o/(2β)$ identified with the TRT odd collision parameter $λ_o$. The TRT may improve stability, accuracy and precision of boundary conditions according to [57]. The free parameter $γ$ (or $λ_o$) is chosen based on the steady state recurrence equations for the TRT evolution [58] but has been tested for simple laminar problems only [59]. The free parameter may also be chosen in order to improve the accuracy of the boundary conditions [60], however, the parametrization is only known for the laminar Poiseuille-flow.
**Regularized LB Model**  The regularized LB scheme (RLB) [16, 47] on the other hand, was proposed to eliminate the influence of higher order moments which may oscillate rapidly and cause numerical instabilities and does not require tuning. In RLB, the relaxation parameters of the ghost moments are chosen such as to annihilate the higher-order non-equilibrium moments in the post-collision state. As any finite lattice representation introduces discrete artifacts among the higher order moment tensors, the regularization operation ensures isotropy, albeit in the confined subspace limited up to the stress tensor level. This is achieved by setting

\[ \gamma_i = 1 \] (2.29)

in Eq. (2.20) for the moments of third order and above. This makes it no longer necessary to store all populations as they are reconstructed from the hydrodynamic variables \( \rho, u \) and \( P \) and thus gives an advantage in terms of memory. On the other hand poor performance at low Reynolds numbers in the lid-driven cavity flow was reported [19] and in our tests in Chapter 7 the RLB was sometimes less stable than LBGK.

**Cascaded Digital LB Model**  The cascaded lattice Boltzmann model (CDLB) [15, 61–63] was introduced because it was found that both LBGK and MRT/TRT are unstable in the limit of large Reynolds numbers (small viscosities) [15]. These instabilities were attributed to violations of Galilean invariance introduced by the choice of the moments in MRT methods [15, 18]. To cure the problem of Galilean invariance, the equilibrium is redefined as a direct discretization of the Maxwellian retaining higher velocity powers [15] to the order supported by the lattice. However, as the Mach number has to be chosen small for incompressible flows, these corrections are minor. It was further stated [15, 18] that the \( D3Q15 \) and \( D3Q19 \) lattices are insufficient and one should resort to the \( D3Q27 \) lattice. More importantly, the central moment representation (2.16) was advocated as to make the process of relaxation Galilean invariant. The name cascaded stems from the dependence of central moments to same and lower order natural moments, see also (2.33) for an example for the \( D2Q9 \) lattice moments. In order to prevent round-off errors, the moments are not relaxed in moment space directly using (2.18)-(2.20) but a truncation operator is used and the post-collision populations are computed by

\[ f' = f + \hat{M}^{-1} m', \] (2.30)
with identical matrix $\hat{M}$ as MRT (2.21) and truncated (digitized) post-collision moments $\hat{m}'$, see also [15] for details. The same authors later identified the coupling of the moments in terms of their underlying macroscopic evolution equations as problematic and proposed and ad-hoc solution [64, 65] which eventually led to the development of the Cumulant LB Model (see next paragraph). The CDLB model is clearly aimed at simulations of turbulence and in [19] the CDLB was tested for the turbulent flow through a flat channel at $Re_\tau = 200$. It was noted that straightforward initialization of the populations as in the LBGK method does not lead to satisfactory results (the same problem was observed for MRT). Nevertheless, the CDLB model remained stable but generated too much artificial viscosity which re-laminarized the flow, unless the Reynolds number was artificially increased.

**Cumulant LB Model** The cumulant lattice Boltzmann model (CLB) [18] is a relatively new method. It is a successor of the CDLB method using the same modified equilibrium, however, the relaxation is carried out in the space spanned by cumulants in order to further disentangle the transport equation for the higher order moments. The transformation to the cumulant space is non-linear, however, and while it allows for the same number of free parameters as the MRT method it does not reduce to the LBGK model for a specific choice of the relaxation constants. The CLB shows promising stability properties [18] but the question how to choose the relaxation parameters remains essentially open.

In summary, performing the process of collision in the dual moment space brings the advantage of individually relaxing different moments with different rates. The choice of the corresponding relaxation parameters is crucial in order to increase the operational range in terms of stability and to achieve accurate results. However, this choice is neither unique nor obvious and often requires careful tuning for specific flow configurations. Although MRT, TRT, CDLB, RLB models were successful in slightly stabilizing the LB method in particular flows, they still remain challenged by high Reynolds numbers and the question how to choose the additional relaxation parameters remains open.
2.4 Moments for standard Lattices

In the following we give explicit expressions for the moment representation of the popular standard lattices which will be used throughout this thesis. For the sake of expressiveness populations $f_i$ are unambiguously re-indexed using tuple and a triple indices, $f_{(j,k)}$ and $f_{(j,k,l)}$, in two and three dimensions, respectively, where $j, k, l \in \{-1, 0, 1\}$ such as to correspond to the microscopic velocity vectors $v_i$ (see also Table 2.1).

2.4.1 Moment Representation for D2Q9

In the sequel, we use the following linear combinations to represent natural moments (2.15)

$$
M_{00}, u_x = M_{10}, u_y = M_{01}, T = M_{20} + M_{02}, N = M_{20} - M_{02}, P_{xy} = M_{11},
Q_{xyy} = M_{12}, Q_{yxx} = M_{21}, A = M_{22}.
$$

(2.31)

These are interpreted as the normalization to the density ($M_{00} = 1$), the flow velocity components ($u_x$, $u_y$), the trace of the pressure tensor at unit density ($T$), the normal stress difference at unit density ($N$), and the off-diagonal component of the pressure tensor at unit density ($P_{xy}$). The (linearly independent) third-order moments ($Q_{xyy}$, $Q_{yxx}$) and the fourth-order moment ($A$) lack a direct physical interpretation for the incompressible flows.

With the set of natural moments (2.31), populations are uniquely represented as follows ($\sigma, \lambda = \{-1, 1\}$):

$$
\begin{align*}
    f_{(0,0)} &= \rho \left(1 - T + A\right), \\
    f_{(\sigma,0)} &= \frac{1}{2} \rho \left(\frac{1}{2}(T + N) + \sigma u_x - \sigma Q_{xyy} - A\right), \\
    f_{(0,\lambda)} &= \frac{1}{2} \rho \left(\frac{1}{2}(T - N) + \lambda u_y - \lambda Q_{yxx} - A\right), \\
    f_{(\sigma,\lambda)} &= \frac{1}{4} \rho \left(A + (\sigma)(\lambda)P_{xy} + \sigma Q_{xyy} + \lambda Q_{yxx}\right). \\
\end{align*}
$$

(2.32)

The natural moments (2.31) can be transformed to their respective central
moments (2.16) using identity

\[ P_{xy} = \tilde{P}_{xy} + u_x u_y, \]
\[ N = \tilde{N} + (u_x^2 - u_y^2), \]
\[ T = \tilde{T} + u^2, \]
\[ Q_{xyy} = \tilde{Q}_{xyy} + 2u_y \tilde{P}_{xy} - \frac{1}{2} u_x \tilde{N} + \frac{1}{2} u_x \tilde{T} + u_x u_y^2, \]
\[ Q_{yyx} = \tilde{Q}_{yyx} + 2u_x \tilde{P}_{xy} + \frac{1}{2} u_y \tilde{N} + \frac{1}{2} u_y \tilde{T} + u_y u_x^2, \]
\[ A = \tilde{A} + 2\left[u_x \tilde{Q}_{xyy} + u_y \tilde{Q}_{yyx}\right] + 4u_x u_y \tilde{P}_{xy} + \frac{1}{2} u^2 \tilde{T} - \frac{1}{2} (u_x^2 - u_y^2) \tilde{N} + u_x^2 u_y^2. \]

Thus, the central moments representation is written upon substituting (2.33) into (2.32) and rearranging terms,

\[ f_{(0,0)} = \rho \left(1 + u_x^2 u_y^2 - u^2\right) + \rho \left(4u_x u_y \tilde{P}_{xy} - \left[\frac{u_x^2 - u_y^2}{2}\right] \tilde{N}\right) + \rho \left(\left[\frac{u^2 - 2}{2}\right] \tilde{T} + 2u_x \tilde{Q}_{xyy} + 2u_y \tilde{Q}_{yyx} + \tilde{A}\right), \]
\[ f_{(0,\sigma)} = \frac{\rho}{2} (u_x^2 + \sigma u_x (1 - u_y^2) - u_x^2 u_y^2) + \frac{\rho}{2} \left(\left[\frac{1 + \sigma u_x + u_x^2 - u_y^2}{2}\right] \tilde{N} - (2\sigma u_y + 4u_x u_y) \tilde{P}_{xy}\right) + \frac{\rho}{2} \left(\left[\frac{1 - \sigma u_x - u_x^2}{2}\right] \tilde{T} - (\sigma + 2u_x) \tilde{Q}_{xyy} - 2u_y \tilde{Q}_{yyx} - \tilde{A}\right), \]
\[ f_{(0,\lambda)} = \frac{\rho}{2} (u_y^2 + \lambda u_y (1 - u_x^2) - u_x^2 u_y^2) + \frac{\rho}{2} \left(\left[\frac{-1 - \lambda u_y + u_x^2 - u_y^2}{2}\right] \tilde{N} - (2\lambda u_x + 4u_x u_y) \tilde{P}_{xy}\right) + \frac{\rho}{2} \left(\left[\frac{1 - \lambda u_y - u_y^2}{2}\right] \tilde{T} - (\lambda + 2u_y) \tilde{Q}_{yyx} - 2u_x \tilde{Q}_{xyy} - \tilde{A}\right), \]
\[ f_{(\sigma,\lambda)} = \frac{\rho}{4} (\sigma \lambda u_x u_y + \sigma u_x u_y^2 + \lambda u_y u_x^2 + u_x^2 u_y^2) + \frac{\rho}{4} \left(4u_x u_y + (\sigma)(\lambda) + 2\sigma u_y + 2\lambda u_x\right) \tilde{P}_{xy} + \left[\frac{-u_x^2 + u_y^2 - \sigma u_x + \lambda u_y}{2}\right] \tilde{N} + \frac{\rho}{4} \left(\frac{u^2 + \sigma u_x + \lambda u_y}{2}\right) \tilde{T} - (\sigma + 2u_x) \tilde{Q}_{xyy} + (\lambda + 2u_y) \tilde{Q}_{yyx} + \tilde{A}. \]
2.4.2 Moment Representation for D3Q27

Analogously to the two-dimensional case, we chose to rename some of the natural moments as reminiscence to their physical meaning:

\[ T = M_{200} + M_{020} + M_{002} \]  \hspace{1cm} (2.35)

is the trace of the stress tensor at unit density,

\[ N_{xz} = M_{200} - M_{002} \]  \hspace{1cm} (2.36)
\[ N_{yz} = M_{020} - M_{002} \]  \hspace{1cm} (2.37)

are the normal stress differences at unit density and

\[ P_{xy} = M_{110} \]  \hspace{1cm} (2.38)
\[ P_{xz} = M_{101} \]  \hspace{1cm} (2.39)
\[ P_{yz} = M_{011} \]  \hspace{1cm} (2.40)

are the off-diagonal components of the stress tensor at unit density. The third order moments lack a direct physical interpretation in the isothermal case but are denoted as 

\[ Q_{xzz} = M_{102}, Q_{xx y} = M_{210}, Q_{yy z} = M_{021}, Q_{xxz} = M_{201}, Q_{yyz} = M_{021} \text{ and } Q_{xyz} = M_{111}. \]

In the basis spanned by the natural moments, populations can be represented as

\[
\begin{align*}
    f_{(0,0,0)} &= \rho [1 - T + M_{022} + M_{202} + M_{220} - M_{222}] \\
    f_{(\sigma,0,0)} &= \frac{1}{6} \rho (3\sigma u_x + 2N_{xz} - N_{yz} + T - 3\sigma Q_{xyy} - 3\sigma Q_{xzz} + 3\sigma M_{122} - 3M_{202} \\
                    &\quad - 3M_{220} + 3M_{222}) \\
    f_{(0,\lambda,0)} &= \frac{1}{6} \rho (3\lambda u_y - N_{xz} + 2N_{yz} + T - 3\lambda Q_{xyy} - 3\lambda Q_{yzz} + 3\lambda M_{212} - 3M_{022} \\
                    &\quad - 3M_{220} + 3M_{222}) \\
    f_{(0,0,\delta)} &= \frac{1}{6} \rho (3\delta u_z - N_{xz} - N_{yz} + T - 3\delta Q_{xxz} - 3\delta Q_{yyz} + 3\delta M_{221} - 3M_{022} \\
                    &\quad - 3M_{202} + 3M_{222}) \\
    f_{(\sigma,\lambda,0)} &= \frac{1}{4} \rho (\sigma \lambda P_{xy} + \lambda Q_{xxx} + \sigma Q_{xyy} + M_{220} - \sigma M_{122} - \lambda M_{212} - \sigma \lambda M_{112} - M_{222}) \\
    f_{(\sigma,0,\delta)} &= \frac{1}{4} \rho (\sigma \delta P_{xy} + \delta Q_{xxz} + \sigma Q_{xxx} + M_{202} - \sigma M_{122} - \delta M_{221} - \sigma \delta M_{112} - M_{222}) \\
    f_{(0,\lambda,\delta)} &= \frac{1}{4} \rho (\lambda \delta P_{yz} + \delta Q_{yyz} + \lambda Q_{xxx} + M_{022} - \lambda M_{212} - \delta M_{221} - \lambda \delta M_{211} - M_{222}) \\
    f_{(\sigma,\lambda,\delta)} &= \frac{1}{8} \rho (\sigma \lambda \delta Q_{xyz} + \sigma M_{122} + \lambda M_{212} + \delta M_{221} + \sigma \lambda M_{112} + \sigma \delta M_{121} \\
                    &\quad + \lambda \delta M_{211} + M_{222}),
\end{align*}
\]

with \(\sigma, \lambda, \gamma \in \{-1, 1\}\). The representation for the central moments is given in the appendix A.1.
Chapter 3

Exact Lattice Boltzmann

Recently there was considerable interest in finding a link between (2.2), using the LBGK mirror state (2.4), and the classical continuous-time kinetic theory in the form of the conventional Bhatnagar-Gross-Krook (BGK) kinetic model,

$$\partial_t f_i(x, t) + v_i \cdot \nabla f_i(x, t) = \frac{1}{\tau} (f_i^{eq}(x, t) - f_i(x, t)),$$

(3.1)

where $\tau$ is the relaxation time. The two fundamental questions here are:

- Is the lattice Boltzmann equation an exact consequence of the classical kinetic theory, and

- Does the over-relaxation follow from the classical kinetic theory (3.1)?

The claim for a positive answer to both questions was given in the influential paper by He, Chen and Doolen (HCD) [66] (see (3.9) below). However, since the approach of HCD used approximations, these questions remained essentially open. The same applies to a more recent analysis [67].

In this section we argue, that the lattice Boltzmann equation (2.2) is a stand-alone discrete time-space dynamical system on its own right and not a discretization of a continuous space-time discrete-velocity kinetic equation. Ignoring this fact has lead to some misinterpretations, for example, of the negative shift in the viscosity as a result of a discretization error. Here we revisit the HCD approach and derive the exact lattice Boltzmann equation using the classical Euler-Maclaurin integration formula. Specifically, we identified therein all contributions responsible for the lattice Boltzmann-type discrete kinetic equation, and have summed up these contributions to all orders. This answers positively the first of the above questions, the LB equation is indeed a direct consequence of the kinetic equation (3.1). However, the exact LB equation does not allow for over-relaxation. In light of these results, the LB
equation with over-relaxation appears as an extension beyond the classical kinetic theory.

### 3.1 Kinetic Equation

We follow He et al. [66] and write the continuous time-space kinetic equation (3.1) along the characteristics, \( x + (v_1 \Delta t)s \), parameterized with a non-dimensional \( s \in [0, 1] \),

\[
\frac{d}{ds} f_i(x + v_1 \Delta ts, t + \Delta ts) = \lambda (f_i^{eq}(x + v_1 \Delta ts, t + \Delta ts) - f_i(x + v_1 \Delta ts, t + \Delta ts)),
\]

where \( \lambda = \Delta t / \tau \), and the local equilibrium,

\[
f_i^{eq}(x + v_1 \Delta ts, t + \Delta ts) = f_i^{eq}[C(x + v_1 \Delta ts, t + \Delta ts)],
\]

depends on space and time through the constraints of local conservation laws \( C \). For example,

\[
\rho(x + v_1 \Delta ts, t + \Delta ts) = \sum_k f_k(x + v_1 \Delta ts, t + \Delta ts),
\]

and similarly for other locally conserved fields. We shall use a short-hand in order to make notation lighter: Let \( T^s_i \) be the shift operator along the characteristics: \( T^s_i \varphi(x, t) = \varphi(x + v_1 \Delta ts, t + \Delta ts) \); Furthermore, we denote \( T_i = T^1_i \) for the shift for the entire time interval \( \Delta t \), and we shall not display space-time dependence \( x, t \) whenever no confusion can happen. We denote \( Q_i = f_i^{eq} - f_i \). Thus, in (3.2) we have

\[
\frac{d(T^s_i f_i)}{ds} = \lambda T^s_i Q_i.
\]

Following He et al. [66], we integrate Eq. (3.4) along its characteristics to get

\[
T_i f_i - f_i = \lambda \int_0^1 T^s_i Q_i ds.
\]

In order to evaluate the integral in (3.5),

\[
I_i = \int_0^1 T^s_i Q_i ds,
\]

HCD [66] used a trapezoidal rule,

\[
I_i \approx \frac{1}{2} (T_i Q_i + Q_i).
\]
With this approximation, Eq. (3.5) becomes
\[ T_i f_i - f_i = \frac{\lambda}{2} ([T_i f_i^{eq} - T_i f_i] + [f_i^{eq} - f_i]). \] (3.8)

This equation is implicit, particularly due to the term \( T_i f_i^{eq} \). HCD were able to eliminate implicitness by a variable transformation, \( f_i = ag_i + (1 - a)g_i^{eq} \), where \( g_i^{eq} = f_i^{eq} \), and the locally conserved quantities are the same for both \( g \) and \( f \). Then, choosing \( a = 2/(2 + \lambda) \), the implicit equation for \( f_i \) becomes explicit for \( g_i \), and is written in terms of the mirror state, \( g_i^* = 2g_i^{eq} - g_i \), as
\[ g_i(x + v_i \Delta t, t + \Delta t) = \left(1 - \frac{\lambda}{2 + \lambda}\right) g_i(x, t) + \left(\frac{\lambda}{2 + \lambda}\right) g_i^*(x, t). \] (3.9)

Functions \( g_i \) can be identified with the populations in the empirical LB equation (2.2). The parametric set of equations (3.9) is equivalent to the family of LB equations (2.2) when \( \lambda \) varies from zero to infinity; in particular it covers the over-relaxation range \( \beta \in [1/2, 1] \) when \( \lambda > 2 \). The above consideration by HCD [66] is elegant; however, it invokes an uncontrolled approximation to evaluate the integral (3.6). Thus, no conclusion can be made regarding the relation between the kinetic equation and the LB equation on the basis of (3.9). Therefore, in the next section we shall evaluate the integral (3.6) without using approximation.

### 3.2 Exact Integration

We now apply the classical Euler-Maclaurin integration formula [see e.g. 68] to evaluate the integral (3.6):
\[
I_i = \frac{1}{2}(T_i Q_i + Q_i) - \sum_{p=1}^{q} \frac{B_{2p}}{(2p)!} \left[ \frac{d^{2p-1}(T_i^s Q_i)}{ds^{2p-1}} \right]_{s=1}^{s=0} - \frac{d^{2p-1}(T_i^s Q_i)}{ds^{2p-1}} \bigg|_{s=0}
\]
\[+ \frac{1}{(2q)!} \int_0^1 B_{2q}(s) \frac{d^{2q}(T_i^s Q_i)}{ds^{2q}} ds, \] (3.10)
where \( B_{2p} \) are (even) Bernoulli numbers, and where \( B_{2q}(s) \) is the Bernoulli polynomial of the order \( 2q \). Here we recognize the trapezoidal rule (first term), followed by the correction terms - the derivatives of the collision integral taken at the ends of the characteristics, and the remainder term.

Derivatives of the collision integral along the characteristics can be written,
\[
\frac{d^p(T_i^s Q_i)}{ds^p} = (-\lambda)^p T_i^s Q_i + \Delta_i^{(p)}, \] (3.11)
where $\Delta_i^{(p)}$ depends on the derivatives of the locally conserved fields along the characteristics. For example,

$$\Delta_i^{(1)} = \sum_{j=1}^{n_c} \frac{\partial f_i^{eq}(C)}{\partial C_j} \frac{d(T_i^s C_j)}{ds}, \quad (3.12)$$

and similar expression for $p > 1$. Functions $\Delta_i^{(p)}$ can be represented using $\Delta_i^{(1)}$ (3.12) as a generating function,

$$\Delta_i^{(p)} = \sum_{k=0}^{p-1} (-\lambda)^{(p-1)-k} \left( \frac{d^k \Delta_i^{(1)}}{d s^k} \right), \quad p > 1. \quad (3.13)$$

Thus, the first term in (3.11) can be termed relaxation-type, while the second term is of the propagation-type. The relaxation-type contributions are the only ones resulting in the lattice Boltzmann part of the Euler-Maclaurin formula, and we shall retain the relaxation-type terms at each order $p$,

$$\frac{d^p (T_i^s Q_i)}{ds^p} \bigg|_{LB} = (-\lambda)^p T_i^s Q_i. \quad (3.14)$$

Propagation-type terms (3.12) and (3.13) which are not retained in the present computation do not lead to the LB-type equation (we shall return to this point below).

Thanks to (3.14), the Euler-Maclaurin formula (3.10) greatly simplifies,

$$I_i = \frac{1}{2} (T_i Q_i + Q_i) + \lambda^{-1} \left( \sum_{p=1}^{q} \frac{\lambda^{2p}}{(2p)!} B_{2p} \right) [T_i Q_i - Q_i] + \frac{\lambda^{2q}}{(2q)!} \int_0^1 B_{2q}(s) T_i^s Q_i ds. \quad (3.15)$$

This allows us to consider the limit $q \to \infty$, and we obtain, instead of (3.7):

$$I_i = \frac{1}{2} (T_i Q_i + Q_i) + \lambda^{-1} B(T_i Q_i - Q_i), \quad (3.16)$$

where $B = \sum_{p=2}^{\infty} B_p \lambda^p / p!$ (odd Bernoulli numbers $B_{2p+1}$ vanish for $p \geq 1$). The above expression is exact (infinite series $B$ is convergent for all $\lambda$). From the generating function of Bernoulli numbers, $\lambda/(e^\lambda - 1) = \sum_{p=0}^{\infty} B_p \lambda^p / p!$, and $B_0 = 1, B_1 = -1/2$ it follows

$$B = (\lambda/2) \coth(\lambda/2) - 1. \quad (3.17)$$

With (3.16) in (3.5) we have, instead of (3.8):

$$T_i f_i - f_i = \frac{\lambda}{2} (T_i Q_i + Q_i) + \left( \frac{\lambda}{2} \coth \left( \frac{\lambda}{2} \right) - 1 \right) (T_i Q_i - Q_i). \quad (3.18)$$
The implicit equation (3.18) differs from the HCD equation (3.8) by the second term in the right hand side, which is not negligible for large $\lambda$. However, implicitness in (3.18) is still of the same type as in (3.8), and can be again removed with a similar transform of variables. Namely, choosing $a = (1 - e^{-\lambda})/\lambda$ in $f_i = a g_i + (1-a) g_i^{eq}$, we transform (3.18) to explicit equation in terms of $g_i$, which renders the result (3.18) in the explicit LB form:

$$g_i(x + v_i \Delta t, t + \Delta t) = \left(1 - \frac{1 - e^{-\lambda}}{2}\right) g_i(x, t) + \left(\frac{1 - e^{-\lambda}}{2}\right) g_i^*(x, t).$$

Thus, by applying the Euler-Maclaurin formula, we integrated the kinetic equation (3.1) along the characteristics in closed form, retaining the LB terms to all orders. In the next section we shall discuss implications of the exact result (3.19).
3.3 Discussion

The general form of the LB equation involving the mirror state can thus be written,

\[ g_i(x + v_i \Delta t, t + \Delta t) = (1 - \varphi(\lambda))g_i(x, t) + \varphi(\lambda)g^*_i(x, t), \tag{3.20} \]

where the function \( \varphi \) maps the parameter \( \lambda = \Delta t/\tau \) onto the LB parameter \( \beta \) in (2.2). In particular, \( \varphi_{EM} = (1 - e^{-\lambda})/2 \) in the Euler-Maclaurin LB equation (3.19) and \( \varphi_{HCD} = \lambda/(2 + \lambda) \) in the HCD (3.9). LB equation (3.20) features over-relaxation if the continuous function \( \varphi \) is monotonic on an interval \([0, \lambda_1]\) (\( \lambda_1 \) can be infinite), \( \varphi(0) = 0 \), and \( \varphi \to 1 \) when \( \lambda \to \lambda_1 \).

Obviously, the exact LB equation (3.19) does not satisfy the said condition since \( \varphi_{EM} \) maps the entire semi-axis \( \lambda \in [0, \infty] \) onto a sub-interval \( \beta \in [0, 1/2] \) only (see Fig. 3.1). The right hand side of Eq. (3.19) is effectively a segment between the state \( g \) and the equilibrium \( g^{eq} \) rather than between \( g \) and the mirror state \( g^* \). Thus, the exact lattice Boltzmann equation (3.19) does not allow the over-relaxation; the over-relaxation domain, \( 1 > \beta > 1/2 \), is disconnected from the kinetic theory domain, \( 1/2 \geq \beta > 0 \).

This is not surprising, as the over-relaxation is precluded by the continuous-time kinetic equation, and we have not relied on any approximation when deriving (3.19). Therefore, any function \( \varphi \approx \) that extrapolates (3.20) into the over-relaxation domain is an extension beyond the result of the kinetic theory (3.19). Hence, there is no unique way to produce such an extension. For example, by the Maclaurin expansion of \( \varphi_{EM} \) we get polynomials \( \varphi_n: \varphi_1 = \lambda/2, \varphi_2 = (\lambda/2)(1 - (\lambda/2)), \varphi_3 = (\lambda/2)(1 - (\lambda/2) + (\lambda^2/6)) \) and so forth. Any odd-degree polynomial, such as \( \varphi_1 \) and \( \varphi_3 \), can be taken as \( \varphi \approx \), with \( \lambda_1 \) found from \( \varphi_n(\lambda_1) = 1 \) (see Fig. 3.1). Finally, let us remind that the viscosity as derived from the kinetic equation (3.1) is \( \nu_K = c_s^2 \tau \). It is interesting to find an extension \( \varphi \approx \) which parameterizes the LB viscosity with the kinetic theory viscosity, \( \nu_{LB} = \nu_K \). In other words, this no-reparametrization condition reads:

\[ (c_s^2 \Delta t/2)(\varphi^{-1} - 1) = \lambda^{-1} c_s^2 \Delta t. \tag{3.21} \]

This implies \( \varphi \approx = \lambda/(\lambda + 2) \), and which is precisely the result of HCD (3.9); in this case \( \lambda_1 \to \infty \). However, apart from this elegant property (no re-parametrization of the viscosity), it is not distinct from other extensions beyond the kinetic theory result (3.19) (see Fig. 3.1).
3.4 Conclusions

To conclude, we have shown that the lattice Boltzmann equation becomes a direct implication of the kinetic theory when the relaxation-type contributions are retained to all orders. To the best of our knowledge, the Euler-Maclaurin integration which was crucial to the derivation of this result was not used in the context of kinetic theory before. The above treatment is applicable to the BGK kinetic model (with a discrete or continuous velocity), which is the core model in the LB context. The result also shows that the resulting exact lattice Boltzmann equation does not feature over-relaxation. In view of this, we have revisited the earlier derivations of the LB scheme based on an approximate treatment, and have demonstrated that they are artifact of the approximation rather than a bridge between the kinetic equation and the lattice Boltzmann equation. The approach of HCD [66] can be a useful recipe to set up the LB equations from the conventional kinetic equations; however, this is a construction method rather than a derivation of LB from kinetic theory.

Finally, the discretization of the BGK kinetic equation using the Euler-Maclaurin formula reveals that the propagation-type terms may eventually lead to novel numerical schemes beyond the standard LB form discussed here. It should be stressed that the LB equation discussed above is the collection of all the relaxation-type terms to all orders, and is the exact LB equation in that sense. Moreover, the relaxation-type terms are dominant at each order in (3.11) close to the hydrodynamic limit. Indeed, the magnitude of the propagation-type term $\Delta_i^{(1)}$ (3.12) is of the order of $\Delta_i^{(1)} \sim \Delta_i C$, where $\Delta_i C$ is the increment of the locally conserved fields (density and momentum) along the $i$th characteristics per one time step $\Delta t$ and one lattice spacing $v_i \Delta t$, and similarly for higher-order terms given by the explicit equation (3.13). Thus, for resolved simulations close to the hydrodynamic limit (large $\lambda$), which always assumes smoothness of the locally conserved fields on the grid scale, the propagation-type terms are indeed small. However, they may become significant for under-resolved simulations, and hence a special attention to these terms has to be paid in such cases.
Chapter 4

Entropic Lattice Boltzmann Method

The second principle of thermodynamics stands out as one of the most general and inescapable laws of physics, with profound bearings on the time evolution of virtually all natural systems [69]. In its essence, it states that any natural system is driven towards a state of maximum entropy (equilibrium), characterized by a maximum number of microscopic configurations. Let us consider the case of an ideal rarefied gas. The dynamics can be described by the Boltzmann equation [70], where the free flight motions of molecules (sustained by kinetic energy) are changed through binary interaction events (controlled by potential energy). Kinetic energy drives the system out of equilibrium, while molecular collisions pull it back to a local equilibrium, in which entropy is locally maximized (Boltzmann's $H$-theorem) [70–72].

While the Lattice Gas supports an analogous $H$-theorem, this property was lost along the way for the lattice Boltzmann equation. The entropic lattice Boltzmann method aims to restore the second law of thermodynamics ($H$-theorem) [20–22, 24], and thus allows for stable and accurate simulations where not all flow scales have been resolved [25–27]. In the following, we describe the main ingredients of the entropic lattice Boltzmann method (ELBM) along with their implications and results. For further details on the ELBM the reader is referred to [50, 73–79]

4.1 Entropic Equilibrium

The entropic lattice Boltzmann method differs from the standard LB in two ways. The first ingredient is to define the local equilibrium through a suitable $H$-function (negative of entropy $S$) consistently with thermodynamics. The
discrete $H$-function \([20, 22]\) reads

\[
H[f] = -S[f] = \sum_i f_i \ln \left( \frac{f_i}{W_i} \right),
\]

which can be viewed as a discretized version of the Boltzmann entropy. The equilibrium is subsequently found as a minimizer thereof under the constraints of local conservation of mass and momentum (and total energy in the case of energy conserving models),

\[
f^\text{eq}_i = \arg\min_f H[f],
\]

s.t. \( \rho = \sum_i f_i, \)

\[
\rho u_a = \sum_i v_{ia} f_i,
\]

which leads to the formal solution,

\[
f^\text{eq}_i = \rho W_i \exp \left[ \chi + \zeta_a v_{ia} \right]
\]

with Lagrange multipliers \( \chi(u) \) and \( \zeta_a(u) \) to be determined upon substitution into the constraints. In the case of the standard lattices a closed form solution can be derived \([22]\) and is written most elegantly in the following product-form (here for the case three-dimensional case):

\[
f^\text{eq}_i = \rho W_i \Psi \left[ B(u_x) \right]^{v_{ix}} \left[ B(u_y) \right]^{v_{iy}} \left[ B(u_z) \right]^{v_{iz}},
\]

where the weights \( W_i \) are

\[
W_i = W_{v_{ix}} W_{v_{iy}} W_{v_{iz}},
\]

\[
W_0 = 2/3,
\]

\[
W_1 = W_{-1} = 1/6,
\]

and function \( \Psi \) is universal for all the discrete velocities (it does not depend on the discrete velocity index),

\[
\Psi(u) = A(u_x) A(u_y) A(u_z),
\]

with

\[
A(u) = 2 - \sqrt{1 + 3u^2}.
\]
Furthermore, the function $B(u)$ contributing to the formation of the last term in (4.4) is written as

$$B(u) = \frac{2u + \sqrt{1 + 3u^2}}{1 - u}. \quad (4.8)$$

Remind that the Maxwellian in $D$ dimensions is written as a product with respect to an arbitrarily fixed Cartesian reference frame, in accord with the familiar property of the shifted Gaussian distribution,

$$e^{-\frac{(v - u)^2}{\theta}} = \left( \prod_{\alpha=1}^{D} e^{-\frac{v^2_{\alpha}}{\theta}} \right) \left( \prod_{\beta=1}^{D} e^{-\frac{u^2_{\beta}}{\theta}} \right) \left( \prod_{\gamma=1}^{D} e^{2u_{\gamma} v_{\gamma}} \right). \quad (4.9)$$

It is easy to recognize the Maxwellian character of the product-lattice equilibrium (4.4) by comparing it to (4.9). The multiplication of the weights in (4.4) corresponds to the first multiplier in (4.9), the function $\Psi$ corresponds to the second multiplier, while the product of functions $B$ reflects the last multiplier in (4.9). However, the true Maxwellian is isotropic, as also revealed by reading equation (4.9) from right to left; the products collapse to a dependence on the kinetic energy in the co-moving frame alone, and the reference to the arbitrarily fixed Cartesian coordinates disappears. This is not so with the discrete velocities. It is imperative therefore to demonstrate that the product-form (4.4) is manifestly isotropic to the order of accuracy of the lattice Boltzmann model. This can be done most elegantly in the following way: Instead of expanding each population (4.4) into powers of the velocity components $u_\alpha$, let us first expand the logarithm of $f_{eq}^i$ (we consider a generic case of dimension $D$ below):

$$\ln f_{eq}^i = \ln \rho + \ln W_i + \sum_{\alpha=1}^{D} \ln A(u_\alpha) + \sum_{\alpha=1}^{D} v_{i\alpha} \ln B(u_\alpha). \quad (4.10)$$

Let us denote $[\varphi(u)]_2$ the operation of the second-order truncation of the expansion of any function $\varphi$ around $u = 0$ to get

$$[\ln f_{eq}^i]_2 = \ln \rho + \ln W_i - \frac{3}{2}(u \cdot u) + 3(v \cdot u), \quad (4.11)$$

where we have used the standard notation,

$$a \cdot b = \sum_{\alpha=1}^{D} a_\alpha b_\alpha, \quad (4.12)$$

for the Cartesian scalar product of $D$-dimensional vectors. Then, using the identity, $[f_{eq}^i]_2 = [\exp(\ln f_{eq}^i)]_2$, we get the same result as Equation (2.13).
The second-order polynomial (2.13) generated by the equilibrium (4.4) is manifestly isotropic, and with the definition of the speed of sound $c_s = 1/\sqrt{3}$ (2.12) it is identical to the standard lattice Boltzmann equilibrium. Thus, both forms of the equilibrium, (4.4) or (2.13), can be used on equal footing for incompressible flows. However, for compressible, trans- and supersonic flows, Equation (4.3) has to be solved numerically in every time step and at every lattice node [31, 32].

4.2 Isentropic Condition

The second ingredient of ELBM consists in redefining the mirror state in order to ensure the discrete-time $H$-theorem:

$$f_{i}^{\text{mirr}} = \alpha f_{i}^{\text{eq}} + (1 - \alpha) f_{i}, \quad (4.13)$$

where the stretch $\alpha$ is found as the non-trivial solution of the isentropic constraint,

$$H[f^{\text{mirr}}] = H[f]. \quad (4.14)$$

Equation (4.14) is non-linear and must be solved numerically at every grid point and in every time step, typically by a Newton-Raphson method. Thanks to convexity of the entropy function, the solution to (4.14) always leads to over-relaxation, $\alpha > 1$.

4.3 Results and Discussion

The entropic estimate $\alpha$ ensures that the entropy is locally always growing, if a solution exists. No solution may be available if the mirror state $f^{\text{mirr}}$ lies in the forbidden region and would imply negative populations. In such a case, the maximally allowed over-relaxation $\alpha_{\text{max}}$ is chosen such that the entropy is maximized. The definition (4.13) leads to a fluctuating relaxation which can be interpreted as as the effective viscosity,

$$\nu_{\text{eff}}(\alpha, \beta) = c_s^2 \left( \frac{1}{\alpha \beta} - \frac{1}{2} \right). \quad (4.15)$$

The entropy-assisted computation thus informs the pre-collision state $f$ about its isentropic mirror $f^{\text{mirr}}$ and stipulates the single condition that the second
law is respected by the post-collision state $f'$. Whenever non-equilibrium effects become strong enough to endanger realizability, the entropic constraint adjusts the relaxation time so as to secure compliance with the second principle. This feedback is self-activated “on demand”, i.e., only whenever and wherever the need arises. And when the danger is gone, most elegantly, the entropic feedback, leaves the stage unsolicited. The second principle decides by itself: sometimes viscosity is increased ($\nu_{\text{eff}} > \nu$) to smooth out sharp features, sometimes it is reduced ($\nu_{\text{eff}} < \nu$) to sharpen the dying ones. In the most demanding cases, the effective viscosity may even drop negative to promote local instabilities and sustain the system against dissipative death.

In Figure 4.1 we illustrate the above by the vorticity field of a flow past a circular cylinder at $Re \sim 3300$, in which many active scales of motion are visible. The Reynolds number, $Re = UD/\nu$, is based on the diameter of the cylinder, which is here taken as $D = 30$, while the mean flow velocity is $U = 0.03$, in lattice units. The computational domain is $9D$ long in the span-wise direction, $35D$ along in the stream-wise direction with $10D$ upstream of the cylinder and $25D$ downstream of it; along vertical direction the domain was $21D$ long with cylinder axis in the mid-plane. We used the lattice with $b = 15$ discrete velocities [23]. Apart from an entropy-supported kinetic equation, we require augmenting boundary conditions that are capable of simulating both resolved and under-resolved flows. Existing boundary conditions such as the bounce-back scheme [6], provide reliable results for resolved simulations but with reducing grid sizes and increasing the Reynolds number, the quality of the simulations is lost due to shock-like instabilities generated at the walls [80]. Hence, we used here the Tamm–Mott-Smith boundary condition [27] (see also Section 5.7.2) for circumventing these instabilities. The flow structures in Figure 4.1a are colored with the effective viscosity, normalized as

$$ R = (\nu_{\text{eff}} - \nu)/\nu. $$

(4.16)

The high quality of resolution of the flow structures (vortex tubes, tangles etc.) is maintained by a concerted action of dampers ($R > 0$) and promoters ($R < 0$). The tiniest structures would not be able to survive unless the effective viscosity is enabled to go negative from time to time, in order to compensate for over-dissipation and “regenerate” small scale structures otherwise doomed by over-damping. Also to be noted (Figure 4.1b) is the spottiness of the effective viscosity, with a highly fine-grained mixing of dampers and promoters. All of the above configures a very elegant preemptive scenario which we can
Chapter 4  Entropic Lattice Boltzmann Method

Figure 4.1: (a) Turbulent flow generated by a round cylinder. Snapshot of the vorticity iso-surfaces are shown, colored with the effective viscosity. Blue: $R > 0$ (dampers); Red/Yellow: $R < 0$ (promoters). The interplay between the dampers and promoters along each vortex tube is clearly visible. (b) Snapshot of the intertwining of dampers ($R > 0$, blue) and promoters ($R < 0$, red). Essential dampers ($R > 1.5$) and promoters ($R < −0.6$) are shown. The entropic feedback is concentrated in the region behind the obstacle, where the transition to turbulence occurs. Gray background: Vorticity.

...take as the hallmark of entropic computing: very attentive “guardian angels”. Amazingly, the spatial pattern of the time-averaged effective viscosity shown in Figure 4.2 resembles indeed a “guardian angel”, protecting the system against numerical crisis.

The ELBM should be viewed as a built-in sub-grid model rather than a mere stabilization technique. Stabilization in ELBM is a by-product of the discrete-time $H$-theorem. Instead of a mere addition of artificial viscosity, the ELBM allows the effective viscosity to fluctuate around the target value $\nu$. In order to clarify this point, note a few general features of the entropic stretch $\alpha$. 
Figure 4.2: Distribution of the time-averaged normalized effective viscosity $R = (\nu_{\text{eff}} - \nu) / \nu$ at the mid-section of the flow past a round cylinder. Red/Yellow: Promoters ($R < 0$); Blue: Dampers ($R > 0$); Green: Nominal ($R = 0$). While the snapshot in Figure 4.1 demonstrates a larger variation of the effective viscosity, the time-average picture is much milder: most of the activity (strongest damping neighboring the strongest promotion) is concentrated at and around the twin shear layers, just behind the cylinder. In the rest of the domain, the deviation of the effective viscosity from its nominal value is less than a fraction of a percent.

**Duality** Let $f$ be a population vector, and $f(\alpha) \equiv f + \alpha(f_{\text{eq}} - f)$ its entropic mirror state, with the same value of the entropy, $H(f(\alpha)) = H(f)$. If the entropy estimate is applied to $f(\alpha)$ instead of $f$, then the initial state is recovered in the form $f = f(\alpha) + \alpha^*(f_{\text{eq}} - f(\alpha))$, with another stretch $\alpha^* > 1$ which satisfies a duality relation:

$$\alpha^* \alpha = \alpha^* + \alpha. \quad (4.17)$$

Equation (4.17) implies that whenever $\alpha \lesssim 2$, the opposite holds for the dual, $\alpha^* \gtrsim 2$. 
The entropic lattice Boltzmann method (ELBM) is a computational method for simulating fluid dynamics that incorporates entropy as a conserved quantity. Chapter 4 of the document focuses on the entropic lattice Boltzmann method (ELBM) and its application to hydrodynamic simulations.

**Evolution and histogram of $\alpha$ for observer point**

The figure shows the evolution of the entropic stretch $\alpha$ at a monitoring point, along with its histogram and a close-up of the histogram around the dominant value $\alpha = 2$.

**Hydrodynamic limit** Whenever the simulation is resolved (populations stay close to the local equilibrium), the stretch $\alpha$ tends to the fixed value $\alpha = 2$ (and so does also the dual stretch, $\alpha^* = 2$, according to (4.17)). Then ELBM self-consistently becomes equivalent to the lattice Bhatnagar-Gross-Krook (LBGK) equation ($\alpha = 2$) and recovers the Navier-Stokes equations with the nominal kinematic viscosity (2.14). Note that the above is a direct implication of the built-in $H$-theorem. Indeed, the resolved simulation, at the kinetic level, is characterized by the fact that all populations are asymptotically close to the local equilibrium. Then, the entropy function becomes well represented by its second-order approximation: at fixed locally conserved fields (density and momentum here), if $\delta f = f - f^{\text{eq}}$, $|\delta f / f^{\text{eq}}| \ll 1$, then $H(f) \approx H^{\text{eq}} + (1/2) \sum_i \delta f_i^2 / f_i^{\text{eq}}$. The levels of the entropy are then asymptotically close to the levels of the above quadratic form. It is under such condition that the entropy estimate (4.14) results in $\alpha = 2$. Note that the standard Chapman–Enskog approximation is valid under precisely the same condition of closeness to the local equilibrium, thereby the viscosity $\nu$ is the same for both ELBM and LBGK.
Effective viscosity and self-averaging  Depending on the outcome for stretch $\alpha$, the effective viscosity $v_{\text{eff}}$ is larger than the viscosity $\nu \equiv v_{\text{eff}}(2\beta)$ if $\alpha < 2$, and it is smaller than $\nu$ if $\alpha > 2$. In the first case, the (larger) effective viscosity leads to smoothing the velocity gradient at the given node, while in the second case, the smaller viscosity leads to a sharpening of the velocity gradient. Note that, when $\beta \to 1$ (vanishing viscosity $\nu \to 0$), the effective viscosity (4.15) can drop to even negative values if $\alpha > 2$. This asymmetry between the over-relaxation being “shorter” ($\alpha < 2$) or “longer” ($\alpha > 2$) than the LBGK over-relaxation $\alpha = 2$ is the crucial implication of the compliance with the $H$-theorem: even if the effective viscosity becomes negative at some lattice nodes, this does not lead to numerical instability because even in that case the $H$-theorem (and the proper behavior of the total entropy) remains valid. The Parameterization with the effective viscosity $v_{\text{eff}}$ can be seen as an alternative to the parameterization with the over-relaxation $\alpha$. Let us note that, if a pair $\{\alpha, \alpha^*\}$ is connected by the duality relation (4.17), then the mean value of the corresponding effective viscosity is equal to the viscosity (2.14),

$$\frac{v_{\text{eff}}(\alpha\beta) + v_{\text{eff}}(\alpha^*\beta)}{2} = v_{\text{eff}}(2\beta) \equiv \nu \quad (4.18)$$

The relation (4.18) is termed self-averaging, and provides important albeit heuristic argument that the averaged-in-time effective viscosity in ELBM simulation is close to the viscosity $\nu$. In other words, we expect that it is only the matter of resolution that the average effective viscosity deviates from $\nu$. This assertion, while not rigorous, is supported by simulation (see Figure 4.2). The rapid fluctuations of the stretch $\alpha$ around $\alpha = 2$ at a given monitoring point chosen at random in the simulation domain are clearly seen in Figure 4.3.

In summary, the ELBGK exploits the self-adaptive mechanism of effective viscosity by choosing automatically the over-relaxation $\alpha$ at each node to guarantee the $H$-theorem at all sites and all discrete time-steps. When the grid is coarsened, over-relaxation $\alpha$ becomes “smeared” in an interval, $[\alpha_{\text{min}}, \alpha_{\text{max}}]$, with $1 < \alpha_{\text{min}} < 2$, and $\alpha_{\text{max}} > 2$. The self-adapted over-relaxation set up by (4.14), results in two oppositely directed effects: if $\alpha < 2$, the effective viscosity is larger than $\nu$, and the ELBM will tend to smoothen any flow perturbation. On the other hand, if $\alpha > 2$, the flow perturbation is enhanced (effective viscosity is smaller than $\nu$). In ELBM simulations, these two effects act simultaneously on various nodes, with the net effect combining stabilization (through smoothing, $\alpha < 2$) with the preservation of the resolution (through sharpening, $\alpha > 2$).
Note that, as $\beta \to 1$, the effective viscosity can even drop to negative values when $\alpha > 2$. This, however, does not lead to instabilities as the total entropy balance remains under control by the discrete-time H-theorem. This all is very different from a conventional perspective on “eddy viscosity” turbulence modelling, and it is not surprising that ELBM does not reduce to familiar large eddy simulation (LES) models [81].

During the last four decades numerous entropic stabilizing techniques have been proposed in computational fluid dynamics (CFD) (see, e.g., Refs [82–90] and references therein). The idea behind is, roughly speaking, to maintain an appropriate amount of artificial viscosity through the analysis of discretization of the entropy balance (physical or artificial). In this regards, ELBM is based on a different premise: it applies to strictly discrete systems (in velocity-space-time), and the discrete-time $H$-theorem does not reduce to the estimate of the entropy production (cf., e.g., [50]).

The closest analog of the conventional stabilization techniques in the LBM setting is perhaps the method of entropic limiters [91–93]. The idea behind is to measure the closeness of the pre-collision state to the corresponding local equilibrium (in the sense of the entropy difference), and to apply equilibration instead of over-relaxation if the difference exceeds a user-defined threshold. This is similar to conventional artificial viscosity stabilization techniques in CFD. Various versions of limiters were considered [91–93]. The authors of [93] claimed that entropic limiters “perform better” than ELBM.

### 4.4 Conclusions

Apart from the simulation of turbulent flows, the entropy feedback has significantly improved stability of thermal flows with temperature gradients [30], multiphase flows [10] and other fluid dynamics problems. This gives us strong confidence that entropy-guidance can be extended to other low-dissipative physical systems.

The second law of thermodynamics provides a parameter-free solution to the problem of controlling the effective turbulent viscosity, so as to tame numerical disruption. Besides turbulence, to which the above findings have an immediate impact on, the general notion of entropy-assisted computing, likely with different realizations of the entropy feedback, is expected to apply to other states of matter characterized by extremely low dissipation, such as superfluids [94] and cosmological fluids [95] near black-hole horizons. It
is also of interest to explore whether a similar paradigm might inform the behavior of active matter systems [96]. Finally, one may extrapolate even further and conjecture that entropy-assisted feedback systems, functioning according to the feedback loop discussed above, may be engineered outside the realm of fluid mechanics, typically at the intersection of information, biology and statistical physics [97–99]. In an even broader perspective, we surmise that entropy-assisted procedures might also inspire the design of novel active feedback systems in natural, biological and possibly also medical sciences.
Chapter 5

Entropic Multi-Relaxation Models

The original LBGK method, Eqs. (2.2),(2.4), is plagued by numerical instabilities when the flow scales are not highly resolved. Thus, the promising nature of LB to simulating low-dissipative systems could not be fully exploited in these early attempts. The MRT and RLB extensions found some remedy to this problem, albeit their success is limited and involves specifically tuned constants. The ELBM on the other hand solved the problem of instability altogether, however, while ELBM converges to LBGK in the resolved case, it locally alters the relaxation parameter which can be interpreted as a modification of the viscosity (4.15).

The main result of this thesis is the development of a new class of LB models (hereafter called KBC models for brevity) which combine the advantages from MRT and ELBM while trying to circumvent their respective disadvantages. That is to say, this long-due lattice kinetic model for high Reynolds numbers comes without the need for tunable parameters or turbulent viscosity and operates at a nominally fixed kinematic viscosity. The resulting KBC models outperform LBGK by orders of magnitude in terms of attainable Reynolds numbers. On the practical side, the analytical formula for the optimal mirror state derived herein adds only a small computational overhead, thus retaining the simplicity, locality and efficiency of LB models.

The key physical principle in its construction dates back to J. W. Gibbs [100] who described optimal (equilibrium) states as points of entropy maximum under relevant constraints. In our case, the optimal mirror states of LB are constructed by maximizing the discrete entropy function (4.1) under the constraints of over-relaxation of the hydrodynamic stresses.

We restrict the remainder of this discussion to standard lattices in two and three dimensions, however, the application of the KBC methodology is valid for any admissible lattice [101].
5.1 Moment Grouping

We redefine the mirror state similarly to the MRT models. Let us first recall, that according to the Eq. (2.18) one can represent the populations as functions of moments. Then we can write,

\[ f_i = k_i + s_i + h_i, \]  
(5.1)

where \( k_i \) (= kinematic part) depends only on the locally conserved fields and the \( s \)-part \( s_i \) (= shear part) necessarily includes the (deviatoric) stress tensor moments,

\[ \mathcal{D} = P - \frac{1}{D} T I, \]  
(5.2)

where \( \rho P = \sum_{i=1}^{q} v_i \otimes v_i f_i \) and \( I \) is the unit tensor. Thus, \( \mathcal{D} \) is a linear combination of the moments \( P_{xy}, N \) and \( P_{xy}, P_{xz}, P_{yz}, N_{xy}, N_{xz} \) in two and three dimensions, respectively (see Section 2.4). The \( s \)-part may also include further non-conserved moments (see the models defined in 5.2 below). Finally, the \( h \)-part \( h_i \) (= higher-order moments) is a linear combination of the remaining higher-order moments not included into the \( s \)-part. Representation (5.1) is easily obtained for any lattice and any moment basis.

With the representation (5.1), a different mirror state can be sought in a one-parameter form,

\[ f_i^{\text{mirr}} = k_i + [2s_i^{\text{eq}} - s_i] + [(1 - \gamma) h_i + \gamma h_i^{\text{eq}}], \]  
(5.3)

where \( \gamma \) is a parameter which is not yet specified and \( s_i^{\text{eq}} \) and \( h_i^{\text{eq}} \) are evaluated at the local equilibrium. We note that, when (5.3) is used in (2.2), one arrives at nothing but a special (not the most general) MRT model of the type considered earlier by many authors for various choices of the moment basis [14, 15, 46]. For any \( \gamma \), the resulting LB model still recovers hydrodynamics with the same kinematic viscosity \( \nu \) (2.14). Note that Eq. (2.2) and Eq. (5.3) can be also rewritten as \( f_i' = f_i + 2\beta(f_i^{\text{GE}} - f_i) \), with the generalized equilibrium [102–104] of the form, \( f_i^{\text{GE}} = f_i^{\text{eq}} + (1/2)(\gamma - 2)(h_i^{\text{eq}} - h_i) \).

The proposal (5.3) is a family of possible mirror states, and the most crucial question is: how to choose the stabilizer \( \gamma \) in order to achieve better performance at small kinematic viscosity \( \beta \to 1 \)? At a first glance, it seems plausible to set \( \gamma = 1 \) (“relax” the higher-order degrees of freedom \( h \) to their equilibrium \( h^{\text{eq}} \); see e. g. [105]). However, in many benchmark flow situations no improvement is achieved. Hence, just the proposal (5.3) is incomplete because it does
not readily answer the above question of how to find an optimal mirror state (5.3).

The over-relaxation of the stresses in the mirror state is the only formal condition to recover the viscosity $\nu$ (2.14), see also Section 5.5. Hence, the major change of perspective here is that the stabilizer $\gamma$ should not be considered as a “tunable” parameter. Rather, it has to be put under entropy control and computed by maximizing the entropy in the post-collision state $f'$. This matches the physics of the problem at hand, since constrained equilibria correspond to the maximum of the entropy (here the constraint is that the stress part remains fixed by the over-relaxation, $s_{\text{mirr}} = 2s_{\text{eq}} - s_i$).

Specifically, let $S(\gamma)$ be the entropy of the post-collision states appearing in the right hand side of (2.2), with the mirror state (5.3). Then we require that the stabilizer $\gamma$ corresponds to maximum of this function. Introducing deviations, $\Delta s_i = s_i - s_{\text{eq}}^i$ and $\Delta h_i = h_i - h_{\text{eq}}^i$, the condition for the critical point reads:

$$\sum_{i=1}^b \Delta h_i \ln \left( 1 + \frac{(1 - \beta \gamma) \Delta h_i - (2 \beta - 1) \Delta s_i}{f_{\text{eq}}^i} \right) = 0. \tag{5.4}$$

Equation (5.4) suggests that among all non-equilibrium states with the fixed mirror values of the stress, $s_{\text{mirr}} = 2s_{\text{eq}} - s_i$, we pick the one which maximizes the entropy. Note that, in this way defined entropic stabilizer $\gamma$ appears not as a tunable parameter but rather it is computed on each lattice site at every time step from Eq. (5.4). Thus, the entropic stabilizer self-adapts to a value given by the maximum entropy condition (5.4). We observe in our simulation that the system entropy is growing over time. It is therefore conjectured that the second law of thermodynamics is approximately fulfilled in practice and moreover, by providing a Lyapunov function, the entropy based relaxation contributes crucially to the stability of the scheme.

In order to clarify the properties of the solution to Eq. (5.4), let us introduce the entropic scalar product $\langle X | Y \rangle$ in the $q$-dimensional vector space,

$$\langle X | Y \rangle = \sum_{i=1}^q \frac{X_i Y_i}{f_{\text{eq}}^i}, \tag{5.5}$$

and expand in (5.4) to the first non-vanishing order in $\Delta s_i / f_{\text{eq}}^i$ and $\Delta h_i / f_{\text{eq}}^i$ to obtain

$$\gamma^* = \frac{1}{\beta} - \left(2 - \frac{1}{\beta} \right) \frac{\langle \Delta s | \Delta h \rangle}{\langle \Delta h | \Delta h \rangle}. \tag{5.6}$$

The result (5.6) explains the mechanism of failure of the proposal $\gamma \approx 1$ at $\beta \approx 1$: Whenever vectors $\Delta s$ and $\Delta h$ are non-orthogonal (in the sense of the entropic
scalar product), the deviation of $\gamma^*$ from $\gamma = 1$ may become very significant. Indeed, in (5.6), the correlation between the shear and the higher-order parts $\sim \langle \Delta s | \Delta h \rangle$ is not a correction to $\gamma = 1$ but rather a contribution of the same order $O(1)$.

## 5.2 Realization in Two and Three Dimensions

The moment grouping (5.1) is discussed here for the natural (2.15) and central (2.16) moment basis. We shall define several realizations of the KBC models by specifying which moments are selected for the $k$-, $s$- and $h$-parts of the populations (5.1). The $k$-part includes the locally conserved moments, $\rho$ and $u$, and is the same for all realizations in their respective moment basis. Any particular model is thus fully specified by the moments retained in the $s$-part (the $h$-part obviously lumps all the moments not included into the $k$- and the $s$-parts). While including the deviatoric stress tensor $\mathcal{D}$ into the $s$-part is mandatory for recovering the Navier-Stokes equations with the correct shear viscosity, the $s$-part may also include other moments provided the basic symmetry properties are not violated. In particular, we consider various combinations of the deviatoric stress $\mathcal{D}$, of the trace of the stress tensor $T = \text{tr}(\mathbf{P})$, and of the third order moment $\mathbf{Q}$ (in the three-dimensional case) to be included into the $s$-part. The explicit form of the dependence on the moments may be easily read off the explicit representations given in Section 2.4 and Appendix A.1.

The kinetically different KBC models for the natural moment representation considered below are as follows: The models KBC-D/KBC-N1 are characterized by the minimal choice of the $s$ part which includes only the deviatoric stress $\mathcal{D}$. By including also the trace of the stress tensor $T$ we get the models KBC-C/KBC-N2. The difference between the former and the latter manifests through a fluctuating bulk viscosity in KBC-D/KBC-N1 while it is fixed for KBC-C/KBC-N2 (see below). Similarly, we define the KBC-N3 model (the $s$-part includes the deviatoric stress $\mathcal{D}$ and the third-order tensor $\mathbf{Q}$) and finally the KBC-N4 model (the $s$-part includes $\mathcal{D}$, $T$ and $\mathbf{Q}$). Note that the kinematic $k$-part is identical for all the four models and the higher-order $h$-part is trivially given as $h_i = f_i - k_i - s_i$.

Similarly, we define KBC variations KBC-B/KBC-C1, KBC-A/KBC-C2, KBC-C3 and KBC-C4 with respect to the central moment basis. The building blocks are now functions of the corresponding central moments. The nomenclature
Table 5.1: Nomenclature key for the KBC models family for central and natural moments. For each model the moments constituting the s-part of the populations $f_i = k_i + s_i + h_i$ are indicated, where $Q$ consists of the moments $Q_{xz}, Q_{xy}, Q_{yz}, Q_{xx}, Q_{yy}$ and $Q_{xyz}$ (and analogously for the central moment $\tilde{Q}$).

<table>
<thead>
<tr>
<th>2D-Model</th>
<th>3D-Model</th>
<th>s-part</th>
</tr>
</thead>
<tbody>
<tr>
<td>KBC-B</td>
<td>KBC-C1</td>
<td>$\tilde{D}$</td>
</tr>
<tr>
<td>KBC-A</td>
<td>KBC-C2</td>
<td>$\tilde{D}, \tilde{T}$</td>
</tr>
<tr>
<td>KBC-C3</td>
<td>KBC-C4</td>
<td>$\tilde{D}, \tilde{Q}$</td>
</tr>
<tr>
<td>KBC-D</td>
<td>KBC-N1</td>
<td>$\tilde{D}$</td>
</tr>
<tr>
<td>KBC-C</td>
<td>KBC-N2</td>
<td>$\tilde{D}, T$</td>
</tr>
<tr>
<td>KBC-N3</td>
<td>KBC-N4</td>
<td>$\tilde{D}, Q$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\tilde{D}, T, Q$</td>
</tr>
</tbody>
</table>

for all the models is summarized in Tab. 5.1. Thus, we consider in total four different KBC models in for $D2Q9$ and eight different KBC models for $D3Q27$, all of which give the same kinematic (shear) viscosity in the hydrodynamic limit but differ in the choice of the s-part and/or in the choice of the moment representation.

### 5.3 Discussion

Figure 5.1 shows an illustration of possible mirror states for LBGK, ELBM and KBC. Here the kinetic space has been projected to the shear $s$ and higher order $h$ moments and a two-dimensional search space is assumed for the sake of illustration. One can observe, that the KBC mirror state in this particular case is found at higher entropy level. However, the opposite case is possible, too. Unlike any MRT, the relaxation parameter $\gamma$ is neither fixed a priori nor is it constant in space and time for KBC models. Therefore, it is instructive to obtain an estimate on the asymptotics for the different models. We restrict this short discussion to the family of two-dimensional KBC models for brevity. Let us expand $\langle \Delta s | \Delta h \rangle$ in powers of velocity $u$,

$$\langle \Delta s | \Delta h \rangle = \langle \Delta s | \Delta h \rangle^{(0)} + \langle \Delta s | \Delta h \rangle^{(1)} + \cdots$$  (5.7)
Figure 5.1: Illustration of the mirror states of KBC, ELBM and the standard LBGK. The dashed lines indicate iso-contours of the constrained convex $H$-function with the local equilibrium at its minimum. LBGK uses a fixed relaxation by over-stepping the equilibrium exactly once. The ELBM searches for a mirror state along the same direction, but applies the isentropic condition $H[f] = H[f^{\text{mirr}}]$. The KBC method uses an over-relaxation for the $s$-part, but searches for the minimum entropy value along the $h$-direction.

At zeroth order this leads to

\[
\langle \Delta s_A | \Delta h_A \rangle^{(0)} = -\frac{1}{4} \rho (9 \tilde{A} - 1)(3 \tilde{T} - 2) \tag{5.8}
\]
\[
\langle \Delta s_B | \Delta h_B \rangle^{(0)} = 0 \tag{5.9}
\]
\[
\langle \Delta s_C | \Delta h_C \rangle^{(0)} = -\frac{1}{4} \rho (9 \tilde{A} - 1)(3 \tilde{T} - 2) \tag{5.10}
\]
\[
\langle \Delta s_D | \Delta h_D \rangle^{(0)} = 0 \tag{5.11}
\]

where we have chosen to replace natural moments by central moments according to (2.33). Note that the two models, B and D, which include the trace of the stress tensor in the higher-order part $h$ do not contribute to the leading order. The next order contributions are
\[
\langle \Delta s_A | \Delta h_A \rangle^{(1)} = 0 \tag{5.12}
\]
\[
\langle \Delta s_B | \Delta h_B \rangle^{(1)} = 0 \tag{5.13}
\]
\[
\langle \Delta s_C | \Delta h_C \rangle^{(1)} = \frac{9}{4} \rho (\tilde{Q}_{xyy} ((2 + 3 \tilde{N} - 3 \tilde{T}) u_x - 12 \tilde{P}_{xy} u_y) - \tilde{Q}_{yxx} (12 \tilde{P}_{xy} u_x \\
+ (-2 + 3 \tilde{N} + 3 \tilde{T}) u_y)) \tag{5.14}
\]
\[
\langle \Delta s_D | \Delta h_D \rangle^{(1)} = -\frac{27}{4} \rho (-\tilde{N} \tilde{Q}_{xyy} u_x + 4 \tilde{P}_{xy} \tilde{Q}_{yxx} u_x + 4 \tilde{P}_{xy} \tilde{Q}_{xyy} u_y + \tilde{N} \tilde{Q}_{yxx} u_y). \tag{5.15}
\]

We see that KBC-B is the only model among the four that does not contribute to either zeroth or first order. This leads to the conjecture that, when \( \beta \rightarrow 1 \), \( \gamma \) will be close to 1 for the KBC-B model, unlike the other KBC models. This is clearly confirmed by our simulation results (see, e.g. figs. 7.3 and 7.5). The average value of the entropic stabilizer \( \gamma \approx 1 \) is found in our simulations for a range of Reynolds numbers and resolutions. Note that by fixing \( \gamma = 1/\beta \) the KBC models coincide with the regularized LB model (more specifically, with a realization of the regularized LB in the according moment basis). Thus, the above theoretical derivation of the entropic stabilizer for model KBC-B produced the empirical regularized LB in the central moment basis. On a related note, KBC model B is also the only model which does not lead to build-up of spurious vortices in the simulation of a perturbed double shear layer, see Section 6.2.

Moreover, evaluations of the entropic stabilizer via solving numerically Eq. (5.4) were found in excellent agreement with the analytical formula (5.6) and have proven to be sufficient for all practical purposes to stabilizing the scheme. The estimate (5.6) it thus used for all the simulations presented in this work unless stated otherwise.

The LB models are valid for high Reynolds numbers rather than for the low ones [6]. This is obvious from the von Kármán relation, \( \text{Re} = \text{Ma}/\text{Kn} \), where \( \text{Ma} = U/c_s \) is the Mach number and \( \text{Kn} = \nu/c_s L \) is the Knudsen number. The hydrodynamic limit is valid at \( \text{Kn} \rightarrow 0 \). Thus, large \( \text{Re} \) implies small deviations from the local equilibrium. Close to the local equilibrium, the entropy in the post-collision state \( \Delta S = S[f'] - S[f_{eq}] \) is a quadratic function (\( \beta = 1 \) for simplicity),

\[
\Delta S(\gamma) = -\frac{(1 - \gamma)^2}{2} \langle \Delta h | \Delta h \rangle + (1 - \gamma) \langle \Delta s | \Delta h \rangle \\
- \frac{1}{2} \langle \Delta s | \Delta s \rangle. \tag{5.16}
\]
Chapter 5  Entropic Multi-Relaxation Models

The maximum of this parabola returns $\gamma^*$ (5.6). If the $\Delta s$ and $\Delta h$ parts happen to be uncorrelated, $\langle \Delta s | \Delta h \rangle = 0$, the entropic stabilizer returns $\gamma = 1$. It is only in this case that the maximum of the entropy in the post-collision state is achieved by the “relaxation”, $h' = h^{\text{eq}}$. However, any correlation between the $s$ and $h$ parts shifts the maximum entropy post-collision state $h'$ away from $h^{\text{eq}}$. Close to the local equilibrium, this shift is simply proportional to the relative strength of the correlation, $\langle \Delta s | \Delta h \rangle / \langle \Delta h | \Delta h \rangle$. The entropy in the maximum entropy state is always higher than in the “relaxed” state:

$$\Delta S(\gamma^*) - \Delta S(1) = \frac{\langle \Delta s | \Delta h \rangle^2}{2\langle \Delta h | \Delta h \rangle} \geq 0. \quad (5.17)$$

These arguments explain why $\gamma^*$ (5.6) is a physically relevant entropy control rather than a mere approximation to (5.4).

5.4  Implementation

The KBC models differ from the standard LBGK in the collision only. For computational efficiency reasons one may rewrite the post-collision state in the form

$$f'_i = f_i - \beta(2\Delta s_i + \gamma\Delta h_i) \quad (5.18)$$

where the higher order moments can be calculated by using the relation $f_i - f_i^{\text{eq}} = \Delta s_i + \Delta h_i$. The resulting operations are given here:

1 compute conserved quantities $\rho, u_\alpha$
2 evaluate equilibrium $f_i^{\text{eq}}(\rho, u_\alpha)$
3 compute $s$ and $s^{\text{eq}}$
4 compute $\Delta s_i = s_i - s_i^{\text{eq}}$
5 compute $\Delta h_i = h_i - h_i^{\text{eq}} = f_i - f_i^{\text{eq}} - \Delta s_i$
6 evaluate $\gamma$ from equation (5.6)
7 relax $f'_i = f_i - \beta(2\Delta s_i + \gamma\Delta h_i)$

The computational overhead of the presented models compared to an implementation with a fixed $\gamma$ is only about 10 percent. If compared to standard LBGK the amount of work is larger as more moments have to be computed additionally which results in an overhead of about $2 - 2.5$ times.
Table 5.2: Second order moments for functions $s$ and $h$ in KBC A-D.

<table>
<thead>
<tr>
<th>Model</th>
<th>$\langle s_i v_{ix} v_{ix} \rangle$</th>
<th>$\langle s_i v_{iy} v_{iy} \rangle$</th>
<th>$\langle s_i v_{ix} v_{ix} \rangle$</th>
<th>$\langle h_i v_{ix} v_{ix} \rangle$</th>
<th>$\langle h_i v_{iy} v_{iy} \rangle$</th>
<th>$\langle h_i v_{ix} v_{iy} \rangle$</th>
</tr>
</thead>
<tbody>
<tr>
<td>KBC A</td>
<td>$\frac{1}{2} \rho (\tilde{T} + \tilde{N})$</td>
<td>$\frac{1}{2} \rho (\tilde{T} - \tilde{N})$</td>
<td>$\rho \tilde{N}_{xy}$</td>
<td>$0$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
<tr>
<td>KBC B</td>
<td>$\frac{1}{2} \rho \tilde{N}$</td>
<td>$-\frac{1}{2} \rho \tilde{N}$</td>
<td>$\rho \tilde{N}_{xy}$</td>
<td>$\frac{1}{2} \rho \tilde{T}$</td>
<td>$\frac{1}{2} \rho \tilde{T}$</td>
<td>$0$</td>
</tr>
<tr>
<td>KBC C</td>
<td>$\frac{1}{2} \rho (T + N)$</td>
<td>$\frac{1}{2} \rho (T - N)$</td>
<td>$\rho \tilde{N}_{xy}$</td>
<td>$0$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
<tr>
<td>KBC D</td>
<td>$\frac{1}{2} \rho N$</td>
<td>$-\frac{1}{2} \rho N$</td>
<td>$\rho \tilde{N}_{xy}$</td>
<td>$\frac{1}{2} \rho T$</td>
<td>$\frac{1}{2} \rho T$</td>
<td>$0$</td>
</tr>
</tbody>
</table>

5.5 Hydrodynamic Limit of KBC Models

Let us derive the hydrodynamic limit of the general kinetic equation with KBC-type mirror state $f^{\text{mirr}}$ (5.3). We will discuss the two-dimensional results here, however, the three-dimensional derivation is analogous. We start by rewriting eq. (2.2) and eq. (5.3) as

$$f_i' = f_i + 2 \beta \left( f_i^{\text{GE}} - f_i \right).$$  \hspace{1cm} (5.19)

with the generalized equilibrium [102–104] of the form,

$$f_i^{\text{GE}} = f_i^{\text{eq}} + \frac{1}{2} (\gamma - 2) (h_i^{\text{eq}} - h_i).$$  \hspace{1cm} (5.20)

In the following derivation, Einstein’s summation convention is applied for all subscript indices except for $i$ where the explicit notation $\langle ... \rangle$ is used. Due to local conservation laws and as a direct consequence of the construction of the moment groups $k$, $s$ and $h$ (see eq. (5.1) and table 5.1) we can immediately state the following relations for the zeroth and first order moments

$$\langle k_i \{1, v_{ia} \} \rangle = \{ \rho, \rho u_a \},$$  \hspace{1cm} (5.21)

$$\langle s_i \{1, v_{ia} \} \rangle = \langle h_i \{1, v_{ia} \} \rangle = 0.$$  \hspace{1cm} (5.22)

While these relations hold for all four KBC models (KBC A-D) discussed here, they depart from each other in the higher order moments. Table 5.2 shows the second order moments for moment functions $s$ and $h$, respectively. Note that all the higher order moments for the kinematic part $k$ vanish.

After the previous preliminary considerations let us expand the left hand side of equation (5.19) using a Taylor series to second order

$$\left[ \delta t (\partial_t + \partial_a v_{ia}) + \frac{\delta t^2}{2} (\partial_t + \partial_a v_{ia}) (\partial_t + \partial_b v_{ib}) \right] f_i = 2 \beta \left[ f_i^{\text{eq}} - f_i + \frac{1}{2} (\gamma - 2) (h_i^{\text{eq}} - h_i) \right].$$  \hspace{1cm} (5.23)
By introducing a characteristic time scale of the flow, $\Theta$, we can rewrite (5.23) in a non-dimensional form using reduced variables $t' = t/\Theta$, $v'_i = v_i/c$ and $x' = x/(c \Theta)$, where $c = 1$. After introduction of the parameter $\epsilon = \delta t/\Theta$ and dropping the primes to simplify notation we get

$$
\left[ \epsilon (\partial_t + \partial_a v_{ia}) + \frac{\epsilon^2}{2} (\partial_t + \partial_a v_{ia}) (\partial_t + \partial_\beta v_{i\beta}) \right] f_i = 2\beta \left[ f_i^{eq} - f_i + \frac{1}{2} (\gamma - 2) (h_i^{eq} - h_i) \right].
$$

(5.24)

By exploiting the smallness of $\epsilon$ we can perform a multiscale expansion of the time derivative operator, the populations and their decomposition into $s$ and $h$ parts until second order,

$$
\epsilon \partial_t = \epsilon \partial_t^{(1)} + \epsilon^2 \partial_t^{(2)} + \cdots
$$

(5.25)

$$
f_i = f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} + \cdots
$$

(5.26)

$$
s_i = s_i^{(0)} + \epsilon s_i^{(1)} + \epsilon^2 s_i^{(2)} + \cdots
$$

(5.27)

$$
h_i = h_i^{(0)} + \epsilon h_i^{(1)} + \epsilon^2 h_i^{(2)} + \cdots
$$

(5.28)

Inserting (5.25)-(5.28) into Eq. (5.24) we can analyze the terms corresponding to orders $\epsilon^0$, $\epsilon^1$ and $\epsilon^2$. The zeroth order terms lead to

$$
0 = 2\beta \left[ f_i^{eq} - f_i^{(0)} + \frac{1}{2} (\gamma - 2) (h_i^{eq} - h_i^{(0)}) \right],
$$

(5.29)

which implies

$$
f_i^{(0)} = f_i^{eq}, \quad h_i^{(0)} = h_i^{eq}.
$$

(5.30)

Local conservation laws dictate the relations $\langle f_i^{eq} \{1, v_{ia}\} \rangle = \langle f_i^{eq} \{1, v_{ia}\} \rangle$ and $\langle h_i^{eq} \{1, v_{ia}\} \rangle = \langle h_i^{eq} \{1, v_{ia}\} \rangle = 0$ which yield the solvability conditions

$$
\langle f_i^{(1)} \{1, v_{ia}\} \rangle = \langle f_i^{(2)} \{1, v_{ia}\} \rangle = \cdots = 0,
$$

(5.31)

$$
\langle h_i^{(1)} \{1, v_{ia}\} \rangle = \langle h_i^{(2)} \{1, v_{ia}\} \rangle = \cdots = 0,
$$

(5.32)

using (5.25)-(5.28).

The terms of order $\epsilon^1$ lead to

$$
(\partial_t^{(1)} + \partial_a v_{ia}) f_i^{eq} = -2\beta \left[ f_i^{(1)} + \frac{1}{2} (\gamma - 2) h_i^{(1)} \right],
$$

(5.33)

from which we can recover the hydrodynamic equations of mass and momentum to first order by taking the zeroth and first order moment of (5.33) and using conditions (5.31) and (5.32) and the definition of $P_{a\beta}^{eq}$ (2.10)

$$
\partial_t^{(1)} \rho = -\partial_a (\rho u_a)
$$

(5.34)

$$
\partial_t^{(1)} u_a = \frac{1}{\rho} u_a \partial_\beta (\rho u_\beta) - \frac{1}{\rho} \partial_\beta P_{a\beta}^{eq}.
$$

(5.35)
Collecting terms of order $\epsilon^2$ results in
\[ [\partial_t^{(2)} + \frac{1}{2} (\partial_t^{(1)} + \partial_a v_{ia})(\partial_t^{(1)} + \partial_\beta v_{i\beta})] f_i^{eq} + (\partial_t^{(1)} + \partial_a v_{ia}) f_i^{(1)} = -2\beta \left[ f_i^{(2)} + \frac{1}{2} (\gamma - 2) h_i^{(2)} \right]. \]

From eq. (5.33) we get the relation
\[ f_i^{(1)} = -\frac{1}{2\beta} (\partial_t^{(1)} + \partial_a v_{ia}) f_i^{eq} + \frac{1}{2} (2 - \gamma) h_i^{(1)}, \] (5.37)
which, once inserted in eq. (5.36), leads to
\[ \left[ \partial_t^{(2)} + \left( \frac{1}{2} - \frac{1}{2\beta} \right) (\partial_t^{(1)} + \partial_a v_{ia})(\partial_t^{(1)} + \partial_\beta v_{i\beta}) \right] f_i^{eq} + \frac{1}{2} (\partial_t^{(1)} + \partial_a v_{ia})(2 - \gamma) h_i^{(1)} = -2\beta \left[ f_i^{(2)} + \frac{1}{2} (\gamma - 2) h_i^{(2)} \right]. \] (5.38)

Taking the zeroth order moment thereof and making use of (5.31), (5.32), (5.34) and (5.35) yields the vanishing second order contribution to the continuity equation
\[ \partial_t^{(2)} \rho = 0. \] (5.39)

The first order moment, however, will render different outcomes for the four KBC models depending on the second order moment of $h$,
\[ \partial_t^{(2)} u_a = \frac{1}{\rho} \left( \frac{1}{2\beta} - \frac{1}{2} \right) \partial_\beta \left( \partial_t^{(1)} P_{a\beta}^{eq} + \partial_\mu Q_{a\beta\mu}^{eq} \right) + \frac{1}{\rho} \partial_\beta \left( (\gamma - 2) \frac{1}{2} \langle h_i^{(1)} v_{ia} v_{i\beta} \rangle \right). \] (5.40)

For models A and C the last term on the right hand side vanishes according to table 5.2 and we get
\[ \partial_t^{(2)} u_a = \frac{1}{\rho} \partial_\beta \left( \left( \frac{1}{2\beta} - \frac{1}{2} \right) \partial_t^{(1)} P_{a\beta}^{eq} + \partial_\mu Q_{a\beta\mu}^{eq} \right), \] (5.41)
while for models B and D one must first analyze the second moment of $h$. As only the trace $\langle h_i^{(1)} v_{ia} v_{i\beta} \rangle$ will contribute we can get the following relation using eq. (5.37), condition $f_i^{(1)} = s_i^{(1)} + h_i^{(1)}$ and table 5.2
\[ \langle h_i^{(1)} v_{ia} v_{i\beta} \rangle = \frac{1}{2} \langle h_i^{(1)} v_{i\mu} v_{i\mu} \rangle \delta_{a\beta} = -\frac{1}{\gamma} \left( s_i^{(1)} + \frac{1}{2\beta} (\partial_t^{(1)} + \partial_\sigma v_{i\sigma}) f_i^{eq} \right) v_{i\mu} v_{i\mu} \delta_{a\beta} \]
\[ = -\frac{1}{2\gamma\beta} \left( \partial_t^{(1)} P_{\mu\mu}^{eq} + \partial_\sigma Q_{\sigma\mu\mu}^{eq} \right) \delta_{a\beta}. \] (5.42)

When inserted in eq. (5.39), this gives the second order contribution to the momentum equation
\[ \partial_t^{(2)} u_a = \frac{1}{\rho} \partial_\beta \left( \left( \frac{1}{2\beta} - \frac{1}{2} \right) \partial_t^{(1)} P_{a\beta}^{eq} + \partial_\mu Q_{a\beta\mu}^{eq} \right) - \frac{1}{2} \left( \partial_t^{(1)} P_{\mu\mu}^{eq} + \partial_\sigma Q_{\sigma\mu\mu}^{eq} \right) \delta_{a\beta} \] (5.43)
For completeness let us now compute the first order terms of the pressure tensor for models A, C and B, D which yield, by substituting the equilibrium values (2.10), (2.11) and using the first order results (5.34) and (5.35)

\[ P_{\alpha\beta}^{(1)} = -\frac{\rho c_s^2}{2\beta} \left[ \partial_\alpha u_\beta + \partial_\beta u_\alpha \right], \quad (5.44) \]

and

\[ P_{\alpha\beta}^{(1)} = -\frac{\rho c_s^2}{2\beta} \left[ \partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{D} \partial_\mu u_\mu \delta_{\alpha\beta} \right] - \frac{\rho c_s^2}{\gamma\beta} \left[ \frac{2}{D} \partial_\mu u_\mu \delta_{\alpha\beta} \right], \quad (5.45) \]

respectively.

By summing up the contributions from first and second order in \( \epsilon \), using (2.10), (2.11), (5.34), (5.35), (5.39) and reintroducing dimensional variables we recover the isothermal Navier-Stokes equations at reference temperature \( T_0 = c_s^2 \)

\[ \partial_t \rho = -\partial_\alpha (\rho u_\alpha), \quad (5.46) \]

\[ \partial_t u_\alpha = -u_\beta \partial_\beta u_\alpha - \frac{1}{\rho} \partial_\alpha (c_s^2 \rho) + \frac{1}{\rho} \partial_\beta \left[ \nu \rho \left( \partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{D} \partial_\mu u_\mu \delta_{\alpha\beta} \right) \right] + \frac{2}{D\rho} \partial_\alpha \left[ \xi \rho \partial_\mu u_\mu \right], \quad (5.47) \]

with the kinematic (shear) and bulk viscosity coefficients

\[ \nu = c_s^2 \left( \frac{1}{\beta} - \frac{1}{2} \right), \quad \xi = \begin{cases} \nu & \text{models A and C} \\ c_s^2 \left( \frac{1}{\gamma\beta} - \frac{1}{2} \right) & \text{models B and D}. \end{cases} \quad (5.48) \]

Note that for the quasi-incompressible LB method the bulk viscosity term is small and can be considered as an artefact of the numerical method. We also point out that the bulk viscosity \( \xi \) for KBC B and D depends on time and space along with the stabilizer \( \gamma \).

### 5.6 Generalization

While (5.3) lumps together all the higher-order moments in the \( h \)-part of the populations, a generalization which makes a distinction within these moments is straightforward: For \( h_i = \sum_m h_{mi} \) with \( m \) labeling the different higher-order moments (or groups of such moments), we have instead of (5.3),

\[ f_{\text{mirr}}^i = k_i + [2s_i^{\text{eq}} - s_i] + \sum_m [(1 - \gamma_m) h_i + \gamma_m h_i^{\text{eq}}] \quad (5.49) \]
while the formula (5.6) generalizes to

$$\gamma_m = \frac{1}{\beta} \left( 2 - \frac{1}{\beta} \right) \sum_n \{C^{-1}\}_{mn} \langle \delta s | \delta h_n \rangle$$  \hspace{1cm} (5.50)

with $C^{-1}$ the inverse of the correlation matrix $C_{mn} = \langle \delta h_m | \delta h_n \rangle$. The generalized KBC method removes essentially the moment basis dependence as the mirror state is found by exploring the full space spanned by the linearly independent moment groups in $h$. The burden of solving (5.50), however, is avoided in the following simulations as the one-parametric KBC models have proven to be sufficient for all (turbulent) benchmark flows.

## 5.7 Boundary Conditions

The treatment of walls and domain boundaries in the lattice Boltzmann method is diverse and reflected by the vast literature on this topic [27, 79, 106–114]. We will restrict this short discussion to the boundary conditions which have shown good conformance with the ELBM as well as with the KBC models [27, 80, 113, 115]. Solely the following boundary conditions are used in the simulations presented in this manuscript.

The general problem consists of finding good approximations for those populations which are missing. Let us define a set $D$ such that $f_i \in D$ are pointing into the fluid region (and are thus missing). This is also illustrated in Figure 5.2 where the missing populations are drawn as dashed arrows. The constraints at the boundary are usually comprised of prescribed target values for the hydrodynamic fields, such as density $\rho_{\text{tgt}}$, velocity $u_{\text{tgt}}$ and occasionally the velocity gradients $\nabla u_{\text{tgt}}$. In order to fulfil these constraints one can either stipulate only the missing $f_i$ or additionally alter the whole distribution.

### 5.7.1 Domain Boundary Conditions

Unless one considers periodic problems, a simulation is spatially confined. At the domain boundaries, the following conditions are usually applied.

**Inflow**

The inflow conditions are typically at fixed density and velocity. Thus, the simplest kinetic condition is to set all populations to their equilibrium value
at target conditions,

\[ f_i = f_i^{\text{eq}}(\rho_{\text{tgt}}, u_{\text{tgt}}) \forall i. \]  

(5.51)

**Outflow**

At the outflow one the target values are usually a priori unknown. In order to solve this problem, one can simply replace the missing populations with their respective values from the previous time step,

\[ f_i(t) = f_i(t-1), \quad i \in D. \]  

(5.52)

**Free-Slip**

In order to mimic an infinite domain, one can simply reflect the out-going populations with respect to the domain normal and thus all the missing populations are defined.

### 5.7.2 Wall Boundary Conditions

In the presence of (curved) walls we consider two boundary conditions. The first is used mainly in earlier simulations while the latter is presently used in most of the simulations (both for KBC and ELBM) for its favourable behaviour.
and the possibility to prescribe velocity gradients. In most cases, a specified target velocity is required at the wall (i.e. no-slip walls) while the target density is unknown. Additionally, the boundary condition should enforce the no-flux condition in wall-normal direction.

**Tamm-Mott-Smith Boundary Condition**

This Tamm-Mott-Smith (TMS) boundary condition [27] involves two steps; a reconstruction and a correction step. First, the target density at the node $x_b$ (see Figure 5.2) is approximated by

$$\rho_{\text{tgt}} = \rho_{\text{bb}} + \rho_s,$$  \hspace{1cm} (5.53)

where $\rho_{\text{bb}}$ is the no-flux density retained after application of the standard (half-way) bounce-back rule, where each missing population is replaced by their point-wise reflection,

$$f_i = \tilde{f}_i, \ i \in D,$$  \hspace{1cm} (5.54)

such that the corresponding microscopic velocities are $v_i = -\tilde{v}_i$. Thus, we have

$$\rho_{\text{bb}} = \sum_{i \in D} f_i + \sum_{i \in D} \tilde{f}_i.$$  \hspace{1cm} (5.55)

The term $\rho_s$ accounts for the mass displacement in case of a moving boundary and is given by

$$\rho_s = \sum_{i \in D} 6W_i \rho_0 v_i \cdot u_w,$$  \hspace{1cm} (5.56)

with reference density $\rho_0$ (here $\rho_0 = 1$) and the wall velocity $u_w$.

The target velocity at the boundary node $x_b$ is estimated by an average among linear interpolations between the previous time step velocity at the fluid node $u_{f,i}$ and the wall velocity $u_w$ for all missing directions by taking into account the respective normalized distance $\Delta q_i$ to the wall (see also Figure 5.2),

$$\mathbf{u}_{\text{tgt}} = \frac{1}{|D|} \sum_{i \in D} \frac{\Delta q_i u_{f,i} + u_w}{1 + \Delta q_i}.$$  \hspace{1cm} (5.57)

The missing populations are subsequently replaced by equilibrium values at the target values

$$f_i = f_{i \text{eq}}(\rho_{\text{tgt}}, \mathbf{u}_{\text{tgt}}), \ i \in D,$$  \hspace{1cm} (5.58)

which concludes step 1.
In the second step a correction force is applied to all populations in order to exactly fulfil the target values at the boundary node $x_b$. This is achieved by computing the current local density $\rho_{\text{loc}}$ and velocity $u_{\text{loc}}$ and applying the TMS force,

$$f_i = f_i + f_i^{\text{eq}}(\rho_{\text{tgt}}, u_{\text{tgt}}) - f_i^{\text{eq}}(\rho_{\text{loc}}, u_{\text{loc}}) \forall i.$$  \hfill (5.59)

**Grad’s Boundary Condition**

The Grad boundary conditions [80, 113, 115] make use of Grad quasi- Equilibrium [116] as an Ansatz for the missing populations, which is given by

$$f_i^*(\rho, u, P) = W_i \left[ \rho + \frac{\rho_{u\alpha} v_{i\alpha}}{c_s^2} + \frac{1}{2c_s^2} (P_{\alpha\beta} - \rho c_s^2 \delta_{\alpha\beta})(v_{i\alpha} v_{i\beta} - c_s^2 \delta_{\alpha\beta}) \right].$$  \hfill (5.60)

The additional dependence on the pressure tensor $P$ makes it possible to incorporate information about the velocity gradients. To this end we use the decomposition $P_{\alpha\beta} = P_{\alpha\beta}^{\text{eq}} + P_{\alpha\beta}^{\text{neq}}$, and estimate the non-equilibrium part from the first-order Chapman-Enskog solution,

$$P_{\alpha\beta}^{\text{neq}} \approx -\frac{\rho c_s^2}{2\beta} \left[ \partial_\alpha u_\beta + \partial_\beta u_\alpha \right].$$  \hfill (5.61)

The missing populations are simply replaced by this Ansatz,

$$f_i = f_i^*(\rho_{\text{tgt}}, u_{\text{tgt}}, P_{\text{tgt}}), \ i \in D$$  \hfill (5.62)

with the target values evaluated as in the TMS boundary condition. The gradients appearing in the non-equilibrium pressure tensor are evaluated with semi-second order finite differences.

In contrast to the TMS boundary conditions, the target values are not exactly enforced on the boundary node $x_b$. The discrepancies are small, however, and the application of this boundary condition has proven advantageous in terms of preventing undesired pressure oscillations and has been successfully applied for many incompressible flow benchmarks [80, 115, 117] as well as for compressible flow simulations (citations needed). Unless stated otherwise, all simulations presented herein use this boundary condition.
Chapter 6

Convergence and Accuracy in the Resolved Limit

This first collection of simulations studied in this thesis is restricted to two-dimensional flows using the D2Q9 lattice. It is imperative at first to thoroughly test the novel KBC models for their accuracy, stability and response to small perturbations and under-resolved cases in the bulk of the fluid flow. In order to exclude the influence of walls and turbulence phenomena, the following benchmark flows feature periodic domains without walls and at moderate Reynolds numbers. The solution to the Green-Taylor vortex flow, the first simulation example, is known analytically and thus we can directly compare the simulation to the theoretical solution. The second array of benchmarks involves a strong shear flow which leads to the formation of two thin shear layers. A small prescribed perturbation causes the shear layers to roll up to form exactly two counter-rotating large vortices which persist for a long time (coherent structures). When reducing the amount of grid points, however, spurious vortices tend to appear in many numerical methods. Thus, these set-ups provide well-founded means to compare the KBC models to theory, the standard LBGK, the entropic ELBM and other numerical methods.

6.1 Green-Taylor Vortex Flow

The KBC scheme is validated for the Green-Taylor vortex flow in a first numerical example. The analytical solution for the Green-Taylor vortex flow is given by

\[ \mathbf{u}(x, y, t) = \nabla \times \left( \frac{\mathbf{u}_0}{k} \cos(k_1 x) \cos(k_2 y) \exp(-v(k_1^2 + k_2^2) t) \right) \]  

(6.1)
Chapter 6  Convergence and Accuracy in the Resolved Limit

\[ \sum_{N} |u_x - \tilde{u}_x| / \sum_{N} |u_x| \]

(a) Convergence rate at \( Re = 10^2, u_0 = 0.03 \).

(b) Convergence at \( Re = 10^3, u_0 = 0.04 \).

\textbf{Figure 6.1:} Convergence rate for Green-Taylor vortex at \( t = t_c \). LBGK (solid black line), KBC A (blue dashed line), KBC B (green cross symbol), KBC C (magenta dotted line), KBC D (orange square symbol), ELBM (red circle symbol), second order convergence (fine dotted line).

where we have chosen \( k_1 = 1, k_2 = 4 \) and the pressure \( p_0 = \rho c_s^2 \) is initialized using \( \rho_0 = 1 \). The populations were initialized using Grad’s approximation (see Equation (5.60)) while the non-equilibrium part (5.61) was pre-computed using the gradients implied by initial condition (6.1). The domain is confined in \( 0 < x, y < 2\pi \) covered by a mesh of \( N \times N \) lattice nodes, the Reynolds number is defined as \( Re = u_0 N / \nu \) and the decay half-time of the flow is given by \( t_c = \ln 2 / \left[ \nu (k_1^2 + k_2^2) \right] \) lattice time steps.

\textbf{Figure 6.2:} Decay of Green-Taylor vortex for times \( t = t_c, 2t_c, 3t_c \) and \( N = 128, Re = 100, u_0 = 0.03 \). Symbols for simulations as in Figure 6.1, analytical solution: light solid. Results represented by symbols have been sub-sampled for clarity.

The Reynolds number was set to \( Re = 100 \) in a first numerical experiment and \( Re = 1000 \) in a second simulation while the initial velocity was \( u_0 = 0.03 \) and \( u_0 = 0.04 \), respectively. Resolution \( N \) was varied between \{64, 128, 256\} in the former and between \{62, 128, 256, 512\} in the latter case. KBC models A-D,
Chapter 6 Convergence and Accuracy in the Resolved Limit

63

LBGK and ELBM were run and compared to the analytic solution. Figure 6.2 shows the decay with time while Figure 6.1 shows the convergence for the relative error at time $t = t_c$. Second order rate is clearly observed for all models, and moreover, all the models are performing almost identically.

6.2 Periodic Double Shear-Layer

To probe the KBC models for their performance in under-resolved simulations of smooth flows with sharp features the doubly periodic double shear layer with a slight perturbation studied extensively in [118] was used as a benchmark. Initial conditions are given by

$$u_x = \begin{cases} u_0 \tanh (\kappa (y/N - 0.25)), & y \leq N/2, \\ u_0 \tanh (\kappa (0.75 - y/N)), & y > N/2, \end{cases}$$

$$u_y = \delta u_0 \sin (2\pi (x/N + 0.25)).$$

Here $N$ is the number of grid points in both $x$ and $y$ directions while periodic boundary conditions are applied in both directions. Grad’s approximation (5.60) was used to initialize the flow field while initial density was set to unity. The parameter $\kappa$ controls the width of the shear layer while $\delta$ is a small perturbation of the velocity in $y$-direction which initiates a Kelvin-Helmholtz instability causing the roll up of the anti-parallel shear layers and is fixed here at $\delta = 0.05$. $u_0$ is the initial magnitude of the $x$-velocity while the Reynolds number is defined as $\text{Re} = u_0 N/\nu$ and the turnover time is $t_c = N/u_0$ lattice time steps.

In [118] it is demonstrated that all the numerical methods investigated therein produce spurious additional vortex roll-ups as a consequence of under-resolution. Effectively no convergence could be reported until the resolution was sufficiently high for the additional vortices to disappear. We pose the question whether the different relaxation for the non-hydrodynamic higher order moments are advantageous for the performance in under-resolved cases. To this end let us consider a thin shear layer case with $\kappa = 80$, $\text{Re} = 30'000$ and $u_0 = 0.04$. We compare KBC models A-D, LBGK and ELBM.

Fig. 6.3 demonstrates a snapshot of the roll up on a fine grid $N = 512$ at time $t = 1t_c$ for the model KBC-A. Here, the solution to (5.4) was found by Newton-Raphson iteration at each lattice node at every time step. While the simulation excellently reproduces the expected shape of the vortex [118], the corresponding snapshot of the spatial distribution of the entropic stabilizer
Chapter 6  Convergence and Accuracy in the Resolved Limit

\( L/2 \quad 0 \quad L/2 \)

\( -L/2 \quad 0 \quad L/2 \)

(a) Snapshot of the vorticity at \( t = 1t_c \).

(b) Distribution of the entropic stabilizer \( \gamma \).

\underline{Figure 6.3:} Roll up of the double shear layer at a grid size of \( N = 512 \) and Reynolds number \( \text{Re} = 30000 \) for model KBC-A.

\( \gamma \) is also shown in Fig. 6.3. It is clear that the entropic stabilizer is far from any fixed value, moreover both positive and negative values of \( \gamma \) are present. Note that, the computed values of the entropic stabilizer \( \gamma \) are not necessarily confined to the so-called linear stability interval \([0, 2]\). This clearly shows that the present new model is far from any LB model with a fixed \( \gamma \), even in a well resolved simulation. Amazingly, as the result of the self-adaptation, the spatial distribution of \( \gamma \) follows the pattern of the developing vortex.

Figure 6.4 shows the vorticity field at \( t = t_c \) for the six schemes under consideration for different resolutions \( N = \{128, 256, 512\} \). LBGK becomes unstable even before \( t = t_c \) is reached (see also fig. 6.6 a) and b)) for \( N = 128 \) while the KBC models deliver stable simulations. In fact, the KBC models are stable all the way up to high Reynold numbers, till at least \( \text{Re} \sim 10^7 \). However, model C and ELBM clearly show formation of additional roll-ups at \( N = 128 \) whereas model D produces comparatively small instabilities. Models A and B (central moments) capture the flow features quite accurately while model B seems to perform slightly better. For the next higher resolution under consideration, \( N = 256 \), LBGK survives but features two small additional vortices while the other models capture the main flow features well. For the largest resolution, \( N = 512 \), all models are essentially indistinguishable.

In summary, KBC-B performs qualitatively better in the under-resolved situation than the other models while for the still slightly under-resolved case, \( N = 256 \), the KBC models and ELBM give comparably good results while LBGK still features spurious vortices at this resolution.
Chapter 6  Convergence and Accuracy in the Resolved Limit

Figure 6.4: Vorticity field at $t = t_c$ for $\kappa = 80$, $u_0 = 0.04$. Columns: LBGK, KBC A, KBC B, KBC C, KBC D, ELBM, respectively, rows: Resolution $N = 128, 256, 512$.

Figure 6.5: Convergence rate for doubly periodic shear layer at $t = t_c$ and $Re = 30000$, $\kappa = 80$, $u_0 = 0.04$. Symbols for simulations as in Figure 6.1, second order convergence (fine dotted). Error with respect to reference solution (LBGK at $N = 2048$ resolution).

These findings are also reflected in figure 6.5 where the second order convergence is reached for all models after $N = 256$. KBC models B and A clearly outperform the other schemes in the under-resolved cases.

Let us now consider the energy and enstrophy decay, depicted in Figure 6.6, where we report both the mean and the fluctuations (r.m.s.) over time. We first remark that the methods converge to each other for $N = 256$ while there is also evidence that the simulation is resolved as the statistics do not change for the next higher resolution, $N = 512$. The energy decay is rather similar for all the models across all resolutions, indicated by both mean and standard
deviation, except for ELBM which shows slightly different results for the mean and fluctuations at $N \leq 128$. The mean enstrophy and fluctuations over time are clearly better captured for the KBC models A, B and D in the under-resolved situation compared to ELBM and KBC C. This is also in accordance with the visual impression of the vorticity structure (fig. 6.4). In summary, the low order statistics seem not affected by the KBC treatment of the higher order moments.

The exceptional stability of the KBC models is attested to the entropy maximisation and it is therefore instructive to monitor the history of the total system entropy $S_{\text{tot}}(t) = \sum_x S[f(x, t)]$ in a domain of $N = 128$. To this end, we select model KBC-A and compare it to ELBM, LBGK and the KBC-A model with fixed

![Figure 6.6](image-url): Evolution of kinetic energy and enstrophy (mean: left axis and large symbols, standard deviation: right axis and smaller symbols). Symbols for simulations as in Figure 6.1, results represented by symbols have been subsampled for clarity.
γ = 1. Figure 6.7 shows that the choice of a fixed second relaxation parameter does not bring any improvement on the stability and leads unbounded decay of $S_{\text{tot}}$ with eventual "blow-up" of the simulation as in the standard LBGK. The entropic models, ELBM and KBC-A, however, are stable and demonstrate monotonic and very similar growth of the total entropy.

**6.3 Conclusions**

In this chapter, two arrays of two-dimensional benchmark simulations are considered at various grid resolutions and Reynolds numbers. The KBC models A-D are compared to ELBM, LBGK and analytical solutions. We first remark, that all the models converge to the LBGK solution for resolved flows and that, in general, the difference among the models under consideration are small and second order rate of convergence is numerically confirmed for all the KBC models for both setups.

At moderately high Reynolds number, the KBC models perform better than LBGK, which suffers from numerical instabilities, and ELBM which produces spurious vortices in the case of the double shear layer. It must be stressed that the entropic models, KBC and ELBM, were stable (in contrast to LBGK) for all the considered cases here and up to very high Reynolds numbers which was attested to the entropy maximisation illustrated by monotonic growth of total entropy.
Among the KBC variations, model KBC-B was demonstrated to be more accurate in the under-resolved shear layer case. The significant difference with respect to the evolution of the stabilizer $\gamma$ for model B may be explained by the orthogonality of the entropic scalar product $\langle \Delta s | \Delta h \rangle$ in the leading and first order terms in velocity powers, see also Section 5.3.
Chapter 7

Decaying Homogeneous Isotropic Turbulence

The deterministic dynamics of the incompressible Navier-Stokes equations may lead to seemingly chaotic behaviour even when starting from smooth initial conditions. This phenomenon is called turbulence and has resisted any analytical description so far. A flow can be characterized by its Reynolds number $\text{Re} = \frac{UL}{\nu}$ and classified into laminar, unsteady and turbulent regimes. With increasing values for $\text{Re}$ the flow becomes more turbulent and the scales of the flow structures (eddies) span an increasing large domain. At large Reynolds numbers, the smallest scales are orders of magnitude smaller than the largest. This makes direct simulations of the Navier-Stokes equations particularly difficult, if not impossible, on current computers. The fundamental questions in turbulence deal with how kinetic energy is dissipated. The famous picture due to Richardson lies at ground of this; kinetic energy associated with large eddies of scale $L$ is transported towards smaller scales by breaking up into smaller eddies until a smallest scale is reached at which the inertial forces are overtaken by viscous forces and dissipation takes effect. This process is also known as energy cascade.

Albeit a consistent theory is still lacking, the most successful quantitative attempt to describe turbulence is due to Kolmogorov [119]. Kolmogorov argued that at this smallest scale (the Kolmogorov length scale $\eta$) the flow is essentially isotropic (without preferential direction) for very high Reynolds numbers. This gave rise to his first universality hypothesis (UH1), which states that the dissipation scale $\eta$ is a function of viscosity $\nu$ and the rate of energy dissipation $\epsilon$ only. By dimensional considerations,

$$\eta = \left(\frac{\nu^3}{\epsilon}\right)^{1/4}, \quad (7.1)$$
where it is assumed that the dissipation rate remains finite, $\epsilon$ is $O(1)$, when viscosity tends to zero $\nu \to 0$ at large Reynolds numbers (viscous anomaly). Kolmogorov further argued, that the inertial motion of eddies which are much smaller than the large scale $L$ but still much larger than the smallest scale $\eta$ is essentially not affected by viscosity. These scales are therefore associated with the internal range, and by dimensional consideration Kolmogorov’s second universality hypothesis (UH2) states that the energy spectrum is a function of the wave vector magnitude $k$ and dissipation rate $\epsilon$ only,

$$E(k, \epsilon) = C k^{-5/3} \epsilon^{2/3}, \quad (7.2)$$

where it is assumed that the eddies in the inertial range are statistically self-similar which implies a statistical scale invariance for larger Reynolds numbers.

These two universality hypotheses have a number of technical implications such as the power-law structure functions. While they give some answers to the long standing problem of turbulence, particularly the second hypothesis UH2 is challenged by experiments and simulations, as there is evidence of non-self-similarity which leads to coherent structures (intermittency).

From the above considerations it is clear that the smallest structures are important and this makes it particularly hard for both simulations and experiments to cope with turbulent flows. When direct numerical approaches are not possible, the effect of the small scales can be taken into account by turbulence models, such as the $k-\epsilon$ model [120], RANS modelling [4] and re-normalization group methods [121], which reduce the computational requirements. However, these models are not universally applicable and have to be selected (and/or tuned) specifically for each flow setup. The lattice Boltzmann, and specifically its entropic variants, may be an efficient alternative way to handle such problems for its combination between hydrodynamics and the microscopic physics [5, 6].

In this chapter, both two- and three-dimensional KBC models are investigated in detail with a particular emphasis on the numerical stability and performance in under-resolved turbulence setups. The different KBC models are compared to ELBM, LBGK and theoretical results. All simulations are carried out in periodic domains without walls and forcing (decaying turbulence). In general, for the simulation of fluid turbulence it useful to study the following questions:

1. is the dynamics of a fully developed turbulent flow accurately captured
Chapter 7  Decaying Homogeneous Isotropic Turbulence

(i.e. initial vortex formation, emergence of coherent structures, vortex-vortex interactions, decay of vortex density)?

2. are near grid-scale structures with large gradients (small vortices) well represented for sufficiently high Reynolds numbers?

3. is the stability affected by the these lattice-scale structures?

4. are low-order statistics well represented and is the numerical scheme correctly modelling the physical dissipation (i.e. decay of energy and enstrophy, scaling laws)?

5. how good is the performance for very large Reynolds numbers in an under-resolved simulation?

7.1 Two-Dimensional Turbulence

Decaying two-dimensional turbulence is characterized by the formation of vortices in the early stage (vortex generation period) which leads to spatially separated coherent structures (which account for the vorticity extrema) which typically have long lifetimes compared to the eddy turnover time and undergo passive advection and vortex-vortex interaction [122]. These vortices can persist, grow over time as they merge with weaker structures of same-sign vorticity and influence the whole field [123]. A large amount of the enstrophy is concentrated within the large-scale vortices that decay slower than

![Figure 7.1: Vorticity field for decaying two-dimensional turbulence Re = 13'134, N = 1024, for LBGK (first row) and KBC B (second row) and times t/t_e = \{10, 20, 40, 60, 80, 100\} from left to right.](image)
Chapter 7 Decaying Homogeneous Isotropic Turbulence

The total energy is roughly constant while enstrophy is decaying. According to [125] the enstrophy follows a direct cascade from large to small scales, much alike the energy cascade in three-dimensional turbulence, while the energy shows an inverse cascade from small to large scales. Classical Kolmogorov-Batchelor scaling theory predicts a slope of $k^{-3}$ and $k^{-1}$ for the energy ($E$) and enstrophy ($Z$) spectrum, respectively, where $k$ is the wave-vector magnitude.

The initial conditions for all subsequent simulations are given by constructing a zero-mean Gaussian random field in Fourier-space with random Fourier-phases and amplitudes proportional to the prescribed spectral density of the stream function $\Psi(k) = k^{-4} Z(k) = k^{-2} E(k)$ from which an incompressible velocity field for a domain of $N \times N$ lattice nodes is obtained. The energy spectral density function is given by

$$E(k) = C_0 k^A \left[ 1 + \left( k/k_0 \right)^B \right]^{-1}$$

where $C_0$ is a normalization constant and the parameters $A = 6$ and $B = 17$ such that the energy spectrum is narrow banded and reasonably peaked at small wave numbers [126].

We consider three groups of numerical experiments. The first simulations are carried out at a moderate Reynolds number $Re = 13'134$ where the energy spectrum was peaked at $k_0 = 9$, the second group was run at $Re = 1.5 \cdot 10^5$ with a different random initial velocity field, $k_0 = 30$, and the last group was simulated at a very high Reynolds number $Re = 1.6 \cdot 10^6$ with the same initial field. Reynolds number is defined as $Re = N \sqrt{2E}/\nu$, where $E$ is the mean initial kinetic energy. A rough estimate of the eddy turnover time is given by $t_e \approx Z^{-1/2}$ [126]. All the simulations were run for 100 $t_e$ in order to observe both vortex formation, merging and decay. The characteristic figures for the initial conditions are summarized in table 7.1. As in all our simulations, Grad’s approximation (5.60) was used to initialize the populations, while here the gradients of velocity were estimated by central differences from the given

<table>
<thead>
<tr>
<th>$N$</th>
<th>256</th>
<th>512</th>
<th>1024</th>
<th>1024</th>
<th>2048</th>
<th>4096</th>
<th>1024</th>
<th>2048</th>
<th>4096</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E(0)$</td>
<td>$1.64 \cdot 10^{-4}$</td>
<td>$1.64 \cdot 10^{-4}$</td>
<td>$1.64 \cdot 10^{-4}$</td>
<td>$1.209 \cdot 10^{-4}$</td>
<td>$1.209 \cdot 10^{-4}$</td>
<td>$1.209 \cdot 10^{-4}$</td>
<td>$1.209 \cdot 10^{-4}$</td>
<td>$1.209 \cdot 10^{-4}$</td>
<td>$1.209 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>$Z(0)$</td>
<td>$8.455 \cdot 10^{-6}$</td>
<td>$2.137 \cdot 10^{-6}$</td>
<td>$5.358 \cdot 10^{-7}$</td>
<td>$3.815 \cdot 10^{-6}$</td>
<td>$9.602 \cdot 10^{-7}$</td>
<td>$2.404 \cdot 10^{-7}$</td>
<td>$3.815 \cdot 10^{-6}$</td>
<td>$9.602 \cdot 10^{-7}$</td>
<td>$2.404 \cdot 10^{-7}$</td>
</tr>
<tr>
<td>$\nu$</td>
<td>$3.533 \cdot 10^{-4}$</td>
<td>$7.066 \cdot 10^{-4}$</td>
<td>$1.413 \cdot 10^{-3}$</td>
<td>$1.062 \cdot 10^{-4}$</td>
<td>$2.123 \cdot 10^{-4}$</td>
<td>$4.246 \cdot 10^{-4}$</td>
<td>$9.52 \cdot 10^{-6}$</td>
<td>$1.990 \cdot 10^{-5}$</td>
<td>$3.981 \cdot 10^{-5}$</td>
</tr>
<tr>
<td>$t_e$</td>
<td>344</td>
<td>684</td>
<td>1366</td>
<td>512</td>
<td>1021</td>
<td>2039</td>
<td>512</td>
<td>1021</td>
<td>2039</td>
</tr>
</tbody>
</table>

Table 7.1: Characteristics for two-dimensional turbulence simulations (lattice units).
initial field. Note that LBGK could not cope with the under-resolved cases \( N = 1024, 2048 \) at \( Re = 1.6 \cdot 10^6 \) and “crashed” due to numerical instabilities where the other five methods run trouble-free.

Let us first consider the low Reynolds number case. Figure 7.1 shows a comparison of the vorticity field for LBGK and KBC B and \( N = 1024 \) at different times. The first column shows the vorticity structures at the point of maximum turbulence activity indicated by the palinstrophy evolution (see fig. 7.3). The vortices have been formed and coherent structures appear in the next shown time instance which interact with each other. The number of vortices is clearly decaying when comparing the last column of fig. 7.1 with the earlier time instances. It is striking that all the models show almost the same dynamics...
Chapter 7  Decaying Homogeneous Isotropic Turbulence

Figure 7.3: Evolution of palinstrophy (left column, mean: left y-axis, large symbols, standard deviation: right y-axis, small symbols) and mean stabilizer $\gamma$, mean entropy $S$ (right column, left y-axis, large symbols and right y-axis, small symbols, respectively) for $Re = 13'134$. Symbols for simulations as in Figure 6.1, results represented by symbols have been sub-sampled for clarity.
Chapter 7  Decaying Homogeneous Isotropic Turbulence

Figure 7.4: Energy and enstrophy spectra for two-dimensional turbulence at Re = 13’134 for N = 1024 at time $t/t_e = 50$. Symbols for simulations as in Figure 6.1, results represented by symbols have been sub-sampled for clarity.

(a) Energy spectrum.  
(b) Enstrophy spectrum.

(for brevity fig. 7.1 shows only LBGK and KBC B). Except for the last time point the plots are visually hardly discriminable. Even after a long time, $t/t_e = 100$, the vorticity structures are still comparable.

The decay of enstrophy was measured and figs. 7.2 b) and d) show the expected exponential decay for resolutions $N = 256$ and $N = 1024$. It is apparent that the evolution of mean enstrophy is the same for all models and is almost identical among the two resolutions. The fluctuations are largely the same, although one can observe a slight flattening at later times for the KBC models compared to ELBM and LBGK for $N = 256$. The evolution of energy, figs. 7.2 a) and c), shows a similar tendency; the models coincide in the mean but differ in the fluctuations for the lower resolution. As all the models are close to each other at $N = 1024$ and the means of enstrophy and energy are not changing compared to $N = 512$ we consider this highest resolution as resolved.

Evidence for this classification is also gathered from figure 7.3 a) and c), where the mean palinstrophy and its fluctuations match for all models at the highest resolution. As stated earlier, at $t/t_e \approx 10$ we observe a peak in palinstrophy which indicates a state of high turbulence intensity. Note that the maximum value is slightly better captured by ELBM and LBGK in the low resolution case.

For all the measured low-order statistical moments we have seen almost identical values, at least in the resolved case, and largely identical mean statistics overall. It is interesting to see, however, that the KBC models differ quite significantly among each other with respect to the evolution of the stabilizer.
Chapter 7 Decaying Homogeneous Isotropic Turbulence

Figure 7.5: Evolution of kinetic energy, enstrophy, palinstrophy and stabilizer γ for \( Re = 1.5 \cdot 10^5 \) at resolution \( N = 4096 \). Mean: left y-axis and large symbols, standard deviation: right y-axis and smaller symbols. Symbols for simulations as in Figure 6.1, results represented by symbols have been sub-sampled for clarity.

\( \gamma \), see fig. 7.3 b) an d). Especially, KBC B is fundamentally different from the other KBC models by γ staying close to 1 all the time. This is consistent with the “quasi-orthogonality” of the \( \Delta h \) and \( \Delta s \) decomposition of this model demonstrated above (see (5.9), (5.13)). Nevertheless, the overall production of entropy is nearly identical for all the considered models.

The scaling of spectral energy and enstrophy density is shown in fig. 7.4 for \( N = 1024 \) and \( t/t_e = 50 \). Due to the moderate Reynolds number the slopes are not expected to match with the theoretical prediction for high Reynolds numbers, however, we are not able to distinguish between the models. Thus we can conclude that for the moderate Reynolds number all methods give
The next simulation was carried out with a higher Reynolds number, \( \text{Re} = 1.5 \cdot 10^5 \), but on a larger grid. The number of initial vortices is much higher due to a different random initial condition. Here we report the results for the highest resolution, \( N = 4096 \). For the lower resolutions, the results are similar, albeit with slightly more variance among the models with respect to the fluctuations of energy.

According to figs. 7.5 and 7.6, where evolution of kinetic energy, enstrophy and palinstrophy as well as spectral density of energy and enstrophy are reported, we observe that the six models behave almost identically. Note that for this Reynolds number LBGK did not encounter any numerical instabilities. Due to the similarities among the models and the fact that the results for \( N = 2048 \) are not significantly different from the largest resolution, we conclude that for \( N = 4096 \) the flow is essentially resolved. Note the differences among the models in figure 7.5 d) for the stabilizer \( \gamma \) which is in accordance with the results from the lower Reynolds number. Although, the Reynolds number here is one order of magnitude higher than before, the scaling of energy and enstrophy is still too steep compared to the theoretical slope.

In order to verify that the discussed models can achieve the proper scaling laws for very high Reynolds numbers, we conducted a simulation at \( \text{Re} = 1.6 \cdot 10^6 \).

Let us first remark that for this highly turbulent regime, LBGK was not able to run with \( N = 1024 \) and \( N = 2048 \). There is evidence that all of the considered
Chapter 7  Decaying Homogeneous Isotropic Turbulence

grids do not fully resolve the flow as the mean statistical quantities are still slightly different among the two highest resolutions, $N = 2048, 4096$, so that the six models are affected differently by the lack of resolution. It is thus interesting to see whether the dissipation is affected by the KBC models in in the presence of under-resolution.

For this matter let us compare the ELBM model and KBC B for the time $t/t_e = 50$ and $N = 4096$. Figure 7.7 shows the vorticity field, accordingly. Note that the all the models produce approximately the same vortex structures up to $t/t_e \sim 20$. Although, one can still see similarities of the structures at $t/t_e = 50$, the two models produce distinctly different pictures. The number of vortices, roughly estimated by the number of vorticity patches exceeding two times the standard deviation of vorticity, is clearly different: ELBM accounts for 3440 whereas KBC B shows 1587 vortices. While visually the number of larger vortices seems comparable, this difference must stem from the very small structures.

These findings are also consistent with the energy and enstrophy spectra depicted in fig 7.9. While ELBM keeps more energy and enstrophy in the large wave numbers, KBC models smoothly fall off. At lower resolution, ELBM shows a bump near the largest wave numbers (see fig. 7.9) which was observed in other simulations as well. This is conjectured to be the effect of the built-in
subgrid model established through the fluctuating effective viscosity. It can be observed, however, that all the models capture the theoretical slope in a range of wave numbers.

On the other hand, the enstrophy evolution, depicted in fig. 7.8 b), shows almost identical average dissipation for all the models at \( N = 4096 \). This indicates that despite the difference in the spectra KBC models do not introduce a significantly higher dissipation, however, it seems that the flux of energy to larger scales is more dominant than in the case of ELBM. Fig. 7.8 a) shows the enstrophy decay for the resolution \( N = 1024 \). Here, the ELBM method clearly shows a slower decay than KBC. When considering the corresponding curve for \( N = 4096 \) and LBGK as a reference (dark dashed line) it is apparent that none of the models capture the expected rate, however, ELBM slightly underpredicts the decay at later times while the KBC models show in general more dissipation (see also fig. 7.9) d) and e)). In contrast to the smallest scales, the large and moderately small scales seem to be predicted well by all methods.

### 7.2 Kida-Vortex Flow

The Kida vortex flow is a well-studied three-dimensional benchmark flow which evolves from a simple deterministic and symmetric initial condition
The Kida vortex flow has been analyzed extensively using DNS [25, 26, 128, 129]. The evolution of enstrophy shows a steep increase in the early stage of the simulation and reaches a maximum value before it decays. For the in a similar process as described by [127].

The Kida vortex flow has been analyzed extensively using DNS [25, 26, 128, 129]. The evolution of enstrophy shows a steep increase in the early stage of the simulation and reaches a maximum value before it decays. For the to a state which resembles a fully developed turbulent flow, which features a corresponding energy cascade. The initial conditions for the flow field are given by

\begin{align}
    u_x(x, y, z) &= U_0 \sin x (\cos 3y \cos z - \cos y \cos 3z) \\
    u_y(x, y, z) &= U_0 \sin y (\cos 3z \cos x - \cos z \cos 3x) \\
    u_z(x, y, z) &= U_0 \sin z (\cos 3x \cos y - \cos x \cos 3y)
\end{align}

where \( x, y, z \in [0, 2\pi] \) and periodic boundary conditions are imposed in all directions. The Reynolds number is defined as \( \text{Re} = U_0 N / \nu \) where \( N \) is the domain size. Initial conditions for the density (and pressure \( p = \rho c_s^2 \)) and higher order moments are obtained by solving the convection-diffusion equation \( \frac{\partial p}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = D \Delta \rho \) on the same grid beforehand until steady state is reached in a similar process as described by [127].

The Kida vortex flow has been analyzed extensively using DNS [25, 26, 128, 129]. The evolution of enstrophy shows a steep increase in the early stage of the simulation and reaches a maximum value before it decays. For the
convergence study we investigate data collected from time points around the peak of enstrophy which indicates the existence of large gradients which are often numerically challenging. A simulation was considered stable if it run until the mean enstrophy,

$$\Omega = \frac{1}{2} \langle \omega \cdot \omega \rangle, \quad (7.5)$$

where vorticity

$$\omega = \nabla \times u, \quad (7.6)$$

was sufficiently decayed ($\Omega / \Omega_0 < 5\%$). Here $\langle \ldots \rangle$ stands for spatial averaging, and $u'$ is the fluctuating part of the flow velocity ($\langle u \rangle = 0$ for Kida vortex),

$$u' = u - \langle u \rangle. \quad (7.7)$$

In order to assess the stability region, the domain size $N = 100$ and initial velocity $U_0 = 0.05$ were fixed and the Reynolds number $Re$ was increased in steps of 500. While LBGK seized to yield sensible values at $Re > 5000$, ELBM was always stable (tested up to $Re = 10^7$). Likewise, all the eight KBC models were always stable, independently of the moment basis or the choice of $s$. This outstanding stability property of all the KBC models, independent of the choice of the moment representation and a particular choice of the $s$- and $h$-partition (moment indifference) has to be contrasted with the so-called “regularized” LB (RLB) method. In the present nomenclature, the eight corresponding RLB models are obtained by fixing $\gamma$ at the outset of the simulation to $\gamma = 1/\beta$. In our benchmark, only the RLB counterpart of the two KBC models, the KBC-N1 and KBC-C1 demonstrated similar stability. All other six RLB models, among them the standard RLB model [16] (the counterpart of the KBC-N2), were less stable than even the LBGK model.

Computational overhead of KBC models compared to the bare LBGK method was ~ 2 times due to computation of additional moments and estimation of stabilizer $\gamma$.

Accuracy of the KBC scheme is studied in detail using Kida vortex flow at $Re = 6000$. The KBC-N4 was used as an example in all further simulations and is compared to LBGK simulation at $N = 600$ (run D) where the flow is considered to be reasonably resolved as indicated by the Kolmogorov length scale $\eta = (v^3/\epsilon)^{1/4} \approx 1.2$ lattice units where

$$\epsilon = \frac{1}{2} \nu \left\langle \left( \frac{\partial u'_a}{\partial x_\beta} + \frac{\partial u'_\beta}{\partial x_a} \right) \left( \frac{\partial u'_a}{\partial x_\beta} + \frac{\partial u'_\beta}{\partial x_a} \right) \right\rangle. \quad (7.8)$$
Chapter 7 Decaying Homogeneous Isotropic Turbulence

Figure 7.10: Iso-surface of vorticity component $\omega_z = 0$ at time $t = 0.5$ colored with velocity magnitude rendered at $z = 0, x, y \in [0, \pi]$ plane. Runs A ($N = 100$), B ($N = 200$), C ($N = 400$) and D ($N = 600$, reference solution).

is the dissipation rate of turbulence kinetic energy. Resolutions $N = 100, 200, 400$ are considered in the following (runs A, B and C, respectively). Convergence towards resolved LBGK simulation is reported in table 7.2 for various statistical quantities. Unless stated otherwise all quantities are given in lattice units. Figure 7.10 shows a comparison of the vortex structures for the four simulations roughly at the point of maximum enstrophy. The vorticity configuration is thus affected by the under-representation of large gradients in the coarse resolutions (see next section). Nevertheless, the large vortex structures are well captured at all resolutions. The largest KBC simulation (run C) is hardly distinguishable from the reference LBGK simulation (run D).

7.2.1 One-Point Statistics

Mean enstrophy $\Omega$ and turbulence kinetic energy

$$k = \frac{1}{2} \langle u' \cdot u' \rangle$$  \hspace{1cm} (7.9)

are important global quantities characterizing the flow and its history. Figures 7.11a and 7.11b, respectively, show the evolution of both quantities with non-dimensional time $t = t_{LB}/(N/U_0)$. It is apparent that in the under-resolved KBC simulations $N = 100, 200$ the enstrophy peak values are not well
Table 7.2: Comparison of LBGK and KBC-N4 for statistical quantities in Kida vortex flow at $Re = \frac{U_0 N}{\nu} = 6000$ and $t = \frac{N}{U_0 t_0} = 0.25, 0.5, 0.75$. Resolutions $N = 100, 200, 400, 600$ for KBC runs A, B, C and resolved LBGK run D, respectively. Convergence rate $p$ of error w.r.t. LBGK solution estimated from polynomial fit ($^*$ indicates exclusion of lowest resolution). All gradient-based quantities are computed by spectral differentiation methods [130]. Turbulence characteristics: length scale $l_0 = k^{3/2}/\epsilon$, velocity scale $u_0 = k^{1/2}$, time scale $\tau_0 = l_0/u_0$, and Reynolds number $Re_0 = l_0 u_0 / \nu$. Taylor characteristics: Taylor micro scale $\lambda = (15v u^2 / \epsilon)^{1/2}$, velocity scale $u_\lambda = u = (2k/3)^{1/2}$ (r.m.s. turbulence intensity), time scale $\tau_\lambda = \lambda/u_\lambda$ and Reynolds number $Re_\lambda = A u_\lambda / \nu$. Kolmogorov characteristics: length scale $\eta = (v^3 / \epsilon)^{1/4}$, velocity scale $u_\eta = (\nu^2 / \epsilon)^{1/4}$ and time scale $\tau_\eta = (\nu / \epsilon)^{1/2}$.

represented. However, for coarse resolutions this is expected. The kinetic energy on the other hand decays quite similarly for all simulations. Table 7.2 reports the numbers at three selected time instances. During simulation, gradients are evaluated using second-order finite differences, which are solely used for reporting the enstrophy evolution in figure 7.11a. All quantities based on gradients in table 7.2 and in the remaining text and figures, however, are computed with spectral differentiation methods [130], unless stated otherwise. This also explains the discrepancies in enstrophy between figure 7.11a and table 7.2 for the lowest resolution $N = 100$.

While the energy seems to be dissipated similarly with time it is important to study the kinetic energy $k$ and dissipation rate $\epsilon$ thereof across flow scales in order to decide whether low-order statistics of turbulent flows yield sensible values in coarse resolution simulations despite the under-representation of
high gradients. The instrument at hand is the spectral representation of the kinetic energy distribution $E(\kappa)$ where $\kappa = |\kappa|$ is the modulus of the wave number vector. Figure 7.12a shows the non-dimensional energy density distribution normalized with kinetic energy

$$k = \int_0^\infty E(\kappa) \, d\kappa. \quad (7.10)$$

According to [119, 131] the energy scales as $E \sim \kappa^{-5/3}$ in the inertial sub-range. The studied Kida flow here does not exhibit large enough Reynolds numbers to see an extended inertial range. However, it is apparent that the energy scales similarly across resolutions and a sharp cut-off is visible at the smallest scales. This indicates that the KBC model is capable of producing the expected energy distribution throughout the scales without an explicit turbulence model. A case for higher Reynolds number shall be examined below.

The cumulative distribution function of the energy-dissipation rate density $D(\kappa) = 2\nu\kappa^2 E(\kappa)$

$$D(\kappa) = 2\nu\kappa^2 E(\kappa) \quad (7.11)$$

illustrates the scales of eddies responsible for the dissipation process, see figure 7.12b. The under-resolved simulations employ expectedly larger eddies for the bulk of the dissipation (see also table 7.2 where the energy dissipation rate $\epsilon = \int_0^\infty D(\kappa) \, d\kappa$ is reported).

The longitudinal skewness factor

$$S_{11}^n = (-1)^n \left\langle \left( \frac{\partial u'_x}{\partial x} \right)^n \right\rangle \left\langle \left( \frac{\partial u'_x}{\partial x} \right)^2 \right\rangle^{-n/2} \quad (7.12)$$
is another global statistical quantity in real space which we report in table 7.2. In agreement with figure 7.11a we find that the outcome of the lowest resolution $N = 100$ is rather inconsistent with the trend observed in the other simulations, however, it agrees well with the resolved case. The lower convergence rate for the odd-order skewness factors may be caused by the inherent lack of isotropy in the third-order moments. However, further studies are needed to draw a concise conclusion.

The remainder of table 7.2 is a compilation of the turbulence, Taylor and Kolmogorov flow scales. Here and with the vast majority of the reported quantities we observe a second-order grid convergence rate, as expected in the context of LB simulations.
7.2.2 Two-Point Statistics

The longitudinal structure function of order $n$ defined as

$$ B_{11}^n = (-1)^n \left\langle \left( \frac{\partial u'_x}{\partial x} \right)^n \right\rangle \left\langle \left( \frac{\partial u'_x}{\partial x} \right)^2 \right\rangle^{-n/2} $$

(7.13)

exhibits linear scaling on logarithmic plots [119, 131]. In particular, the second order structure function scales as $B_{11}^2 \sim r^{2/3}$. Figure 7.13a depicts the results with the theoretical scaling. Due to the relatively low Reynolds number we may not identify an extended inertial range but we note that the simulations agree well with the reference over the entire range of $r$.

Another real-space two-point statistical quantity that can be used to assess different numerical techniques is the correlation of the velocity field. Here the longitudinal and transverse correlation functions are defined as

$$ \rho_{11}^n (r) = \frac{\left\langle u'_x(x, y, z) u'_x(x + r, y, z) \right\rangle}{\left\langle u'_x(x, y, z) u'_x(x, y, z) \right\rangle} $$

(7.14)

$$ \rho_{22}^n (r) = \frac{\left\langle u'_y(x, y, z) u'_y(x + r, y, z) \right\rangle}{\left\langle u'_y(x, y, z) u'_y(x, y, z) \right\rangle}. $$

(7.15)

A comparison at time $t = 0.5$ is given in figure 7.13b. All simulations with $N \geq 200$ show excellent agreement with the reference solution. At the maximum distance $r = 0.5$ the velocity components are still correlated which is associated with the low Reynolds number (see figure 7.16b for comparison).
7.2.3 Stabilizer $\gamma$ and the LBGK Limit

The importance of the self-adjusting stabilizer $\gamma$ becomes clear when considering its evolution in time and its distribution in space. In fact, the evolution of $\gamma$ is closely correlated with the flow field (see Figure 7.14a). In the regions of higher turbulence intensity it is distinctly different in the mean and shows larger fluctuations. Figure 7.14a depicts the spatial variation of $\gamma$ for the simulations A, B and C. For the run A (the coarsest resolution) the variations of the stabilizer are large but diminish subsequently when resolution is increased. Note that for $N = 400$ a large part of the domain governed by $\gamma \sim 2$ (green areas). The distribution of $\gamma$ in space reveals the close relation of $\gamma$ to the flow as can be seen by the superimposed vorticity magnitude contours in figure 7.14a.

In general, we observe that when the spatial resolution is increased the mean of stabilizer tends to the value $\gamma = 2$ and shows significantly smaller fluctuations. For the discussion in this and the next sections, we executed a control run (run E hereafter) on the grid $N = 600$ with the selected KBC-N4 model, that is, with the same resolution as for the LBGK simulation of the run D. Figure 7.14b shows the mean stabilizer $\langle \gamma \rangle$ at $N = 100$ and $N = 600$ (runs A and E, respectively), together with its standard deviation. It is apparent that $\langle \gamma \rangle$ is far from being constant in the low resolution case, whereas $\langle \gamma \rangle = 2$ and fluctuations around the mean value are tight (but not negligible) for the highest resolution (run E). This gives yet another indication of convergence towards the LBGK model which has a fixed value of $\gamma = 2$. It is remarkable that the LBGK limit $\gamma = 2$ is found for all the eight KBC models in this and other three-dimensional simulations (this is at variance with the two-dimensional case, see [2]). While we defer analytical proof of this statement based on the equation (5.6) to a separate study, it is important to observe that the KBC models automatically tend to the LBGK limit once the resolution is increased. This feature (achieving the LBGK limit) of the KBC models is similar to the known property of the standard entropic LB (ELBM), and is different from any MRT model with a priori fixed relaxation times.

7.2.4 Convergence to the Navier-Stokes Equations at Small Scales

In the previous sections convergence of KBC models towards LBGK was demonstrated through various low-order statistical quantities, as well as by
the analysis of the stabilizer. Table 7.3 shows the relative difference of selected statistical quantities between the two reasonably resolved simulations on the grid of same size $N = 600$, run D (LBGK) and run E (KBC-N4). The majority of the quantities are within a margin of 0.5% throughout the range of time (around the peak turbulence intensity). This shows that the two models produce almost identical results at sufficiently large resolutions.

A slightly larger difference ($\sim 1\%$) is reported for the mean enstrophy $\Omega$ and the dissipation rate $\epsilon$ which are directly dependent on the gradients in the system. The origin of these differences may be explained by considering compliance with the constraint of incompressibility, $\nabla \cdot u = 0$. As the lattice Boltzmann method is weakly compressible, i.e. the pressure field is imposed by equation of state and not by solving the pressure-Poisson equation, this is of general interest regarding the quality of a simulation. Figure 7.15 shows the root mean square of the divergence of the velocity for the runs D and E. It is apparent that the LBGK model leads to a slightly larger compressibility as compared to the KBC on the grid of same size. This can be attributed to the fluctuations of the stabilizer $\gamma$ in the KBC model which still persist even when the mean has reached the LBGK value $\langle \gamma \rangle = 2$ (see Figure 7.14b). Note that the mean of the divergence, $\langle \nabla \cdot u \rangle$, vanishes for all the models. It is also noted that KBC models which allow for a fluctuating bulk viscosity are even less compressible than both LBGK and the KBC models with the fixed bulk viscosity, especially for low resolution.

While the energy cascade and the evolution of the low-order statistics show the trends which one would expect from a realization of the incompressible flow,

<table>
<thead>
<tr>
<th>time</th>
<th>0.25</th>
<th>0.5</th>
<th>0.75</th>
<th>1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$</td>
<td>0.09672</td>
<td>0.1957</td>
<td>0.1581</td>
<td>0.5773</td>
</tr>
<tr>
<td>$u'$</td>
<td>0.04835</td>
<td>0.09782</td>
<td>0.07901</td>
<td>0.2891</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>0.2747</td>
<td>0.4154</td>
<td>1.009</td>
<td>0.9649</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>0.2663</td>
<td>0.4166</td>
<td>1.006</td>
<td>0.9674</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>0.08461</td>
<td>0.1100</td>
<td>0.4206</td>
<td>0.1967</td>
</tr>
<tr>
<td>$Re_\lambda$</td>
<td>0.0363</td>
<td>0.01232</td>
<td>0.342</td>
<td>0.09292</td>
</tr>
<tr>
<td>$\eta$</td>
<td>0.06647</td>
<td>0.1039</td>
<td>0.2499</td>
<td>0.2433</td>
</tr>
</tbody>
</table>

Table 7.3: Relative difference in percentage of statistical quantities in Kida vortex flow at $Re = \frac{U_0 N}{\nu} = 6000$ for times $t = \frac{N}{U_0} = 0.25, 0.5, 0.75, 1.0$ and resolution $N = 600$ for LBGK (run D) and KBC (run E).
it is still of interest to quantify the recovery of the Navier-Stokes equations at small scales. To that end, let us remind that the incompressible Navier-Stokes equation implies the following balance equations for the averaged momentum, vorticity, energy and enstrophy which yield for statistically homogeneous flows [132, 133],

\[
\begin{align*}
\partial_t \langle u \rangle &= 0, \\
\partial_t \langle \omega \rangle &= 0, \\
\partial_t k &= -2\nu \Omega, \\
\partial_t \Omega &= \langle \omega \cdot s \cdot \omega \rangle - 2\nu P,
\end{align*}
\]

where

\[
s = \frac{1}{2} (\nabla u + \nabla u^\dagger),
\]

is the rate-of-strain tensor, and \( P \) is the palinstrophy,

\[
P = \frac{1}{2} \langle \nabla \omega : \nabla \omega \rangle.
\]
Table 7.4: Effective viscosity ratio $\nu_{eff,k}/\nu$ for simulations A, B, C and E at different time instances.

<table>
<thead>
<tr>
<th>time</th>
<th>0.25</th>
<th>0.5</th>
<th>0.75</th>
<th>1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>run A</td>
<td>1.5971</td>
<td>1.5210</td>
<td>1.5640</td>
<td>1.4698</td>
</tr>
<tr>
<td>run B</td>
<td>1.1173</td>
<td>1.1507</td>
<td>1.1356</td>
<td>1.0595</td>
</tr>
<tr>
<td>run C</td>
<td>1.0303</td>
<td>1.0311</td>
<td>1.0030</td>
<td>0.9302</td>
</tr>
<tr>
<td>run E</td>
<td>0.9875</td>
<td>1.0039</td>
<td>0.9976</td>
<td>0.9005</td>
</tr>
</tbody>
</table>

In the simulation, the Navier-Stokes equation will be verified at small scales if the ratio $\nu_{eff}/\nu \approx 1$. Thus, evaluation of effective viscosities (7.22) and (7.23) is an important check of the accuracy, which is also used in the standard CFD methods.

Eqs. (7.16), (7.17), (7.22) and (7.23) are evaluated for simulations A, B, C and E where the time and space derivatives are computed with fourth-order accurate central differences and spectral differentiation, respectively. The effective viscosity ratio based on the energy balance (7.22) is reported in Tab. 7.4. By increasing the resolution the values are approaching $\nu_{eff,k}/\nu \approx 1$. It is apparent that even for the coarsest run A the additional dissipation is rather small which is consistent with the evolution of turbulence kinetic energy $k$ shown in Fig. 7.11b. Note that at the highest resolution, the effective viscosity fluctuates around the target value $\nu$, with lower values (that is, with a higher effective Reynolds number). The second effective viscosity $\nu_{eff,\Omega}$, reported in table 7.5, is considerably larger for simulations A and B which is expected from comparison to the mean enstrophy dynamics shown in figure 7.11a. However, for larger resolutions the values are close to the nominal viscosity.

Thus, we conclude that the KBC scheme recovers well the Navier-Stokes equations for reasonable resolutions while introducing only small additional dissipation at coarse grid simulations. We also note that we have not found a consistency check as above done on other available LB models in the literature.
Table 7.5: Effective viscosity ratio $\nu_{\text{eff},\Omega}/\nu$ for simulations A, B, C and E at different time instances.

<table>
<thead>
<tr>
<th>time</th>
<th>0.25</th>
<th>0.5</th>
<th>0.75</th>
<th>1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>run A</td>
<td>2.2622</td>
<td>2.2577</td>
<td>2.0950</td>
<td>1.8545</td>
</tr>
<tr>
<td>run B</td>
<td>1.2603</td>
<td>1.4505</td>
<td>1.4042</td>
<td>1.3943</td>
</tr>
<tr>
<td>run C</td>
<td>1.0575</td>
<td>1.1120</td>
<td>1.0912</td>
<td>1.0776</td>
</tr>
<tr>
<td>run E</td>
<td>1.0282</td>
<td>1.0474</td>
<td>1.0337</td>
<td>1.0383</td>
</tr>
</tbody>
</table>

Figure 7.16: Turbulence kinetic energy spectrum and longitudinal and transversal velocity correlation functions at $\text{Re}_\Lambda = 564$, $t = 0.075$ (solid) and initial values at $\text{Re}_\Lambda = 2000$ (dashed).

7.3 Large Reynolds Numbers

The second three-dimensional numerical example is the simulation of a highly turbulent flow starting from a random initial condition and decaying with time. The periodic and cubic domain with box-length $N = 400$ was initialized with a flow field generated from a prescribed narrow-banded initial energy spectrum peaked at grid wave-number $\kappa N = 8$,

$$E_0 = 400 \left(\frac{2}{3}\right)^{1/4} \left(2\nu u'_0^3 / \pi \right)^{1/2} b^2 k^4 \exp \left[-b k^2 \right],$$

where $\nu = 8.164970 \cdot 10^{-5}$ and $u'_0 = 0.01$. The initial values of the density (and pressure) and the higher order moments were generated with the same procedure as described earlier for the Kida flow.

The main objective is to test the KBC scheme for an under-resolved simulation (Kolmogorov scale $\eta \approx 10$ lattice units) at large Reynolds numbers ($\text{Re}_\Lambda \approx 600$).
In particular, we ask whether the scheme is stable for a random and highly turbulent flow in absence of a deterministic and highly symmetric initial condition, whether low-order statistics are well represented and physical dissipation (i.e. scaling laws) is modeled correctly. By means of this simulation we examine the general question of the performance for large Reynolds numbers in an under-resolved simulation from yet another point of view. While a resolved simulation was not attempted, we compare our results to the classical scaling laws.

Figure 7.16a shows the turbulence kinetic energy spectrum at $t = t_{LB}/(N/u'_0) = 0.075$. The inertial range is extended and the scaling is more apparent than in the less turbulent simulations above. The sharp cut-off at the smallest scales is still maintained despite the coarse resolution. As before, numerical stability is naturally guaranteed to very high Reynolds numbers. While the initial spectrum is narrow and steep, it flattens during the course of energy decay and exhibits the Kolmogorov scaling in the inertial sub-range roughly at peak of mean enstrophy. Figure 7.16b shows the velocity correlations where the contributions to the correlations are vanishing for $r/N > 0.2$ at $t = 0.075$. Hence, the velocity field is largely uncorrelated as one would expect from isotropic homogeneous turbulent flows. While these results are far from a comprehensive study, they contribute to the overall assessment that the KBC scheme might perform well even in the case of severe under-resolution. A more comprehensive investigation shall be conducted in a further study.

### 7.4 Conclusions

The simulation of two- and three-dimensional homogeneous isotropic turbulence was chosen as a benchmark to assess various statistics for high Reynolds numbers. Stability and accuracy was studied in detail and compared to LBGK, ELBM and theory. Minor differences in performance among the different KBC versions are observed for different simulations, however, all KBC models are much more stable than LBGK. This demonstrates that the KBC approach is quasi moment-indifferent, unlike other versions of MRT models. The KBC models were shown to capture the expected scaling laws for energy and enstrophy spectra in the case of high Reynolds numbers. Low order statistics such as averages and fluctuations of kinetic energy, enstrophy, palinstrophy and rate of dissipation as well as the spectral densities for energy,
enstrophy and rate of dissipation agree well with resolved simulation despite the under-resolution. Second-order rate of convergence was numerically confirmed in the vast majority of the statistical quantities of interest and all the KBC models considered here have the correct limit of LBGK for resolved simulations.

There is indication that the KBC models produce less small structures than ELBM (and LBGK) for the under-resolved cases, however, the decay of enstrophy is only slightly accelerated in the two-dimensional under-resolved case for high Reynolds numbers. On the other hand ELBM tends to somewhat amplify the appearance of small structures which lead to a slight over-representation of enstrophy (and energy) content at large wave numbers but only for very coarse resolutions.

In general, we showed that by keeping the kinematic (shear) viscosity coefficient constant (in contrast to ELBM) the presented method is extremely stable and produces accurate results in the presence of under-resolution. On the other hand, the KBC models introduce additional computational overhead in order to compute additional moments and the estimate for the stabilizer $\gamma$ which accounts for not more than a factor of $2 - 2.5$ for both two and three dimensions.

These findings and the parameter-free and explicit nature of KBC as well as the lack of explicit turbulence modelling renders the scheme a promising candidate for applications in both research and engineering contexts were high Reynolds numbers and computational cost are of importance.
Chapter 8

Complex and Wall-bounded turbulent Flows

In this chapter the KBC models are applied to three dimensional flows in the presence of walls and at challenging Reynolds numbers which gives rise to a complex interplay between shear flows, boundary layers, turbulence phenomena and large vortex structures as often encountered in engineering problems. On the one hand, the boundary conditions for curved walls are put to the test here, but on the other hand, the KBC models are evaluated in terms of their performance in under-resolved (almost) real world problems. In particular, we pose the question whether the KBC models can deliver sensible results for low-order statistics at coarse resolutions.

To this end, we study the turbulent flow in a channel and in a round pipe, as well as the flow around a bluff body (circular cylinder) and the flow around a reference car model at high Reynolds number.

Further simulations using KBC-N1 model not presented here are the turbulent flow in an engine-like geometry [117] and the flow around a sphere using block grid refinement [134].

8.1 Turbulent Channel Flow

As a first example of homogeneous wall-bounded turbulence simulations the standard benchmark of the turbulent channel flow is chosen. The flow is characterized by the Reynolds number

$$Re_t = \frac{u_t h}{v} \quad (8.1)$$
based on the wall friction velocity $u_t$ and channel half-width $h$. The wall friction velocity is defined as

$$u_t = \sqrt{\frac{\tau_w}{\rho}}, \quad (8.2)$$

with the shear stress at the wall in normal direction,

$$\tau_w = \rho \nu \frac{\partial u_x}{\partial y} \bigg|_{y=0} \quad (8.3)$$

with the main flow directed along the $x$-axis and the wall located at $y = 0$. Based on the above definitions, one can introduce the following dimensionless wall units [135],

$$x^+ = \frac{x u_t}{\nu},$$

$$u^+ = \frac{u}{u_t}, \quad (8.4)$$

for space and velocity, respectively. Assuming that the average flow velocity depends only on the distance to the flat wall in a homogeneous turbulent flow and using similar considerations as Kolmogorov, von Kármán [136] introduced the famous log-law of the wall,

$$u^+(y^+) = \kappa^{-1} \log y^+ + C^+, \text{ for } y^+ \gg 1, \quad (8.5)$$

with the von Kármán constant $\kappa \approx 0.41$ and $C^+ \approx 5.5$. While this relation is phenomenological it is extensively confirmed by experiments and simulations. A channel half-width $h = 50$ lattice units is used in the following simulations with extents of $20h$ and $3h$ in stream-wise and periodic transverse direction, respectively. After an initial transient phase, statistics were accumulated for $\sim 4 \cdot 10^6$ time steps. In order to drive the flow the approach by [27] was followed, where a body force $g$ is used, and introduced in the kinetic equation by the exact-difference method [137],

$$f'_i = (1 - \beta) f_i(x, t) + \beta f_{i}^{\text{mirr}}(x, t) + F_i, \quad (8.6)$$

where

$$F_i = f_i^{\text{eq}}(\rho, u + \Delta u) - f_i^{\text{eq}}(\rho, u), \quad (8.7)$$

with the velocity increment $\Delta u = g \Delta t$. In the simulation, the Reynolds number is not known a priori, but can be estimated from the average flow profile at
Figure 8.1: Instantaneous vortex structures in the turbulent channel flow at $\text{Re}_\tau = 180$ (KBC-C2).

The channel center [27] which leads to

$$g_x = \frac{\text{Re}_\tau^2 v^2}{h^3}. \quad (8.8)$$

The effective Reynolds number can be checked a posteriori by either directly measuring the wall shear stresses (8.3) from a resolved simulation, or by comparing the relation of the average flow velocity at channel center to the log-law of the wall (8.5) which results in an implicit equation for the effective $u_\tau$, see also [27] for more details.

The first simulation was run at a moderate Reynolds number $\text{Re}_\tau = 180$. The non-dimensional grid spacing $\Delta^+ = \frac{\Delta x u_\tau}{v}$ is typically used as a measure of resolution which leads to $\Delta^+ \approx 3.5$. The results are compared to the DNS data of Moser et al. [138] where a non-uniform grid is used leading to $\Delta^+ \approx 0.1$ at the wall. Figure 8.2 shows the comparison of the KBC-C2 model to the DNS data for both the mean flow velocity in stream-wise direction as well as for all r.m.s. velocity fluctuations. Agreement is excellent, especially in the log-law regime despite the rather coarse resolution with only two grid points in the viscous sub-layer.

The identical flow setup and domain was subsequently used to simulate the turbulent channel flow at $\text{Re}_\tau = 590$. This leads to severe under-resolution with $\Delta^+ \approx 10$. The mean flow, however, is still predicted accurately as shown
(a) Average stream-wise velocity.
(b) R.m.s. velocity fluctuations.

**Figure 8.2:** Average stream-wise velocity and r.m.s. velocity fluctuations in wall units in the simulation of the turbulent channel flow at $Re_\tau = 180$. Symbol: KBC-C2; Solid line: DNS data [138]. The log-law of wall (dashed) is shown to guide eye.

(a) Average stream-wise velocity.
(b) R.m.s. velocity fluctuations.

**Figure 8.3:** Average stream-wise velocity and r.m.s. velocity fluctuations in wall units in the simulation of the turbulent channel flow at $Re_\tau = 590$. Symbol: KBC-C2; Solid line: DNS data [138]
in Figure 8.3a. The Reynolds stresses (r.m.s. velocity fluctuations) are slightly under-predicted but overall in good agreement with the DNS data.

8.2 Turbulent Pipe Flow

The next wall-bounded turbulent flow considered here, the flow through a round pipe, adds the complexity of curved walls. An illustration of the instantaneous vortex structures is shown in Figure 8.4. This problem has been studied extensively in the literature experimentally, analytically and numerically. While for the flat channel there is consensus about the scaling of the mean velocity profile, it is less clear for the turbulent flow through a pipe and is being discussed in the literature (see, e.g., [139–147]). Nevertheless, there exists reliable DNS and experimental data. Here we choose a Reynolds number $Re_D = 5300$ based on the pipe diameter $D$ and the mean bulk velocity $\overline{u_{\text{bulk}}}$, same as in the DNS of [147].

As the problem is axially symmetric, it is conveniently formulated in cylindrical
coordinates and one typically uses a corresponding computational mesh. The classical LB method, however, is restricted to a rectilinear Cartesian mesh. Thus, this benchmark problem is probing the performance of the boundary condition for curved walls to its full extent as the flow is wall bounded.

Three simulations are conducted at diameter $D = \{49, 99, 199\}$ lattice units (runs A, B and C). The domain length in stream-wise direction is $L = 16R$ where $R = D/2$ is the pipe radius. The flow is initialized with a random velocity field and evolved for $200\; T$, where the turnover time is given by $T = R/\overline{u_{\text{bulk}}}$. After this initial transient, statistics are collected for another $200\; T$, yielding a total run-time of $400\; T$. The pressure gradient was adjusted during the simulation to reach the desired Reynolds number, which was realized through a body force as given by Eq. (8.7). The corresponding von Kármán number is $R^+ = u_t R/\nu = 180$ with the wall friction velocity $u_t$ and the kinematic viscosity $\nu$.

The distance from the pipe wall is given by $R - r$ with $r = \sqrt{x^2 + y^2}$ where $z$ denotes the spatial coordinate in stream-wise direction. The non-dimensional wall units employed hereafter, see Eq. (8.4). Thus, the non-dimensional distance to the wall is $(R - r)^+ = R^+ - r^+$. A natural measure for spatial resolution is the non-dimensional and uniform grid spacing $\Delta x^+$ here, while for the DNS

---

**Figure 8.5:** Mean velocity component in flow direction for the turbulent pipe flow. KBC-N1.
Figure 8.6: Rms velocity profiles for the turbulent pipe flow. See Fig. (8.5) for the legend.
of [147] radial ($\Delta r^+$), azimuthal ($\Delta(r\theta)^+$) and stream wise ($\Delta z^+$) directions are varying non-uniformly. The finest resolution for the DNS is typically found at the wall in the wall-normal direction. In [147] this amounts to $\Delta r^+|_{r=R}=0.167$ (with a maximum $\Delta r^+|_{r=0.409R}=1.647$), while in our simulations $\Delta x^+=7.3$ (run A), $\Delta x^+=3.6$ (run B) and $\Delta x^+=1.8$ (run C).

Fig. (8.5) shows the comparison of the mean stream-wise velocity component of runs A-C to the reference DNS results. Despite severe under-resolution excellent agreement can be observed for runs B and C. Run A obviously employs a mesh which is too coarse to capture the scaling of the mean correctly.

The next order statistical moments are depicted in Figs. (8.6a-8.6d). The r.m.s. fluctuations of the axial, radial and azimuthal velocity component show the same trend as seen in Fig. (8.5); the coarsest simulation does not reproduce the expected values while runs B and C are very close to the DNS results. Moreover, the cross-correlations of the axial and radial fluctuations, Fig. (8.6d), show excellent agreement for simulations B and C, as well.

### 8.3 Flow around circular Cylinder

The KBC model is tested for the well-studied flow around a circular cylinder. The computational setup is depicted in Figure 8.7, where a uniform inflow profile at $U = 0.05$ is used and periodic boundaries in the span-wise $z$-direction. The Reynolds number $Re = UD/\nu$ is based on the diameter $D$. In order to mimic an infinite domain in $y$-direction a large extent of $20D$ was chosen with free-stream boundaries. The cylinder was placed sufficiently far from inlet and outlet to minimize the effect of the boundaries.

**Figure 8.7:** Simulation set-up for the flow past a circular cylinder with diameter $D$. 
The first set of simulations was run at low to moderate Reynolds numbers up to \( \text{Re} = 500 \) in order to evaluate the forces exerted on the body (drag forces) and the shedding frequency (Strouhal number). To this end, two resolutions were chosen, \( D = \{10, 20\} \). The averaged results are compared to experimental data and shown in Figure 8.8. The agreement is good for both the mean drag coefficient \( C_D \) and the Strouhal number \( St \).

At high Reynolds numbers it is no longer possible to achieve correct predictions for the aerodynamic coefficients unless a highly refined grid is used in order to resolve the boundary layer. Nevertheless, the flow velocity profile in the vicinity and in the wake of the cylinder may be still accessible. The Reynolds number was subsequently increased to \( \text{Re} = 140000 \) for a cylinder diameter \( D = 30 \) lattice units. In addition, the span-wise domain was increased to the width of \( 5D \) and TMS boundary conditions were applied. The results were compared with PIV measurements of the near-wake velocity field at the same Reynolds number reported in [153]. In Figs. 8.9a-8.9d the mean velocity and r.m.s. velocity fluctuations contours are are overlapped with the experimental data of Ref. [153]. Despite the obvious under-resolution which makes it impossible to correctly measure drag, the low-order velocity statistics agree surprisingly well with the experimental data. The location of the recirculation zones are predicted well
as seen from Figs. 8.9a and 8.9c and also the size and onset of the shear layer is captured reasonably well, see also Figs. 8.9b and 8.9d.

8.4 Flow around a reference Car Model

In this section we investigate the performance of the KBC model on a relevant engineering flow around a generic car model at high Reynolds number. The simple car model under consideration here originates from the early experimental works of Morel [154] and Ahmed [155–158], which led to the quasi-standardization of a simplified generic model with a slanted back, generally referred to as "Ahmed body". In particular, the wake structures, separation characteristics and the drag as a function of the slant angle were studied in
detail. The drag was found to be largest at a critical angle of 30° while a steeper slant leads to a more significant detachment of the flow at the rear with a large recirculation zone. Below the critical angle, the flow reattaches at the slant, resulting in two dominant counter-rotating longitudinal vortices along the slant edges reaching far into the wake.

This flow has attracted considerable interest and has been extensively studied in further experiments [159–166] and simulations using different numerical methods such as LES [167–173], DES [174], RANS [175, 176] and URANS [177, 178]. A LB simulation with refinement, relaxation time limiters and $k - \varepsilon$ turbulence model can be found in [179]. In addition, the flow around the Ahmed body was used as a test case for turbulence models in two ERCOFTAC workshops [180, 181].

![Diagram of the Ahmed body](image1)

(a) Geometry of the Ahmed body [158].

![Simulation set-up](image2)

(b) Simulation set-up for the flow around the Ahmed body with dimensions $L_B = 1590$, $W_B = 601$, $H_B = 450$, $d_B = 690$ in lattice units.

**Figure 8.10:** Dimensions of the reference car and the computational domain.

The original dimensions of the model used in the wind tunnel tests are given in Figure 8.10a, with length $L = 1044$ mm, height $H = 288$ mm, width $W = 389$ mm and the radius $R = 100$ mm of the rounded front part. The length
of the slanted back is $d_1 = 222$ mm inclined at an angle $\varphi = 25^\circ$. Instead of wheels, the car model uses four cylindrical posts; the front pair is at a distance $d_2 = 202$ mm from the strut, and the rear pair is located after a spacing of $d_3 = 470$ mm. The posts are displaced by $d_4 = 163.5$ mm from the symmetry plane and the ground clearance is $d_5 = 50$ mm.

We compare our results to the experiments carried out by Lienhart et al. [160] who used a Laser-Doppler anemometer technique to measure mean and fluctuations of the flow velocity around and in the wake of the car. The slant angle here is $\varphi = 25^\circ$ with a Reynolds number $Re = u_\infty L/\nu = 2.7 \cdot 10^6$ based on the length of the car.

In the simulation with KBC-N4, the length of the car $L$ was resolved with 300 lattice units and a uniform inflow velocity of $u_\infty = 0.05$ was used. Dimensions of the computational domain are depicted in Figure 8.10b. In order to mimic an unbounded domain the free-slip boundary was used at the top domain boundary, while periodic boundary conditions are applied in $y$-direction. Note, that a uniform Cartesian grid is employed without any refinement. It is clear, that with such a coarse grid the boundary layer cannot be resolved and thus accurate prediction of the aerodynamic coefficients is not possible. The mean velocity and its fluctuations, however, are predicted quite accurately as shown in the next paragraph.

In Figure 8.11a and 8.11b the mean flow in stream-wise and vertical direction is shown at the symmetry plane $y = 0$, while Figure 8.11c shows the corresponding vector field. The agreement of the simulation with experiment is excellent apart from the regions close to the wall at the top rear surface of the car which can be attributed to the low resolution. The next three Figs. 8.11d-8.11f show three components of the Reynolds stress tensor (r.m.s. fluctuations) for the same plane. Small deviations from the experiments are visible above the slant, however, the overall agreement is quite good.

In general the flow in front of the car is captured excellently and the largest discrepancies are expectedly found close to the slant where the flow reattaches. Further downstream in the wake the match is again very good.

This is also confirmed by Figs. 8.12a-8.12f where the velocity vector field $(u_y, u_z)$ is shown at selected planes perpendicular to the main flow direction at the rear end and in the wake of the car. In particular, the location and strength of the longitudinal counter-rotating vortices is captured with very good agreement to the experiment by [160]. The deflection of the vortex tubes down and inwards is clearly visible which is one of the main characteristics of
selected case with a slant angle of $\phi = 25^\circ$.

### 8.5 Further Applications

The KBC model, in particular model KBC-N1, was used to simulate an array of further simulations of complex flows in the works of our collaborators Benedikt Dorschner and Nicolò Frapolli. Here we present a short overview in order to demonstrate the performance of KBC in canonical and challenging other turbulent flow set-ups.

#### 8.5.1 Flow past Sphere

Dorschner et al. [134] carried out the canonical flow around a sphere at Reynolds number $Re = U D / \nu = 3700$ (based on sphere diameter $D$). A uniform inflow and periodic boundary conditions in the perpendicular directions to the main flow are used. The domain is block-wise refined near the sphere with a maximum refinement of $D = 120$. Mean drag coefficient $C_d$, the averaged base pressure coefficient $C_{pb}$, the recirculation length $L_r$, and the separation angle $\phi_s$ as well as mean velocity profiles and the pressure coefficient distribution are compared with experiments, DNS and LES simulations, see also Figure 8.13. The results agree very well with the literature for all measured quantities. It is also pointed out in [134] that the average flow velocity profiles could have been captured using a uniform (non-refined) coarse resolution, however, the near-wall features require high spatial resolution.

#### 8.5.2 Flow in Engine-like Geometry

A detailed study of the turbulent flow in a simplified internal combustion engine with an open valve and a moving piston at 200 rpm with a maximum Reynolds number $Re_{\text{max}} = 3070$ based on the piston speed and the cylinder diameter was attempted in Dorschner et al. [117] using a uniform grid. Multiple intake cycles were simulated and cycle-to-cycle variability and formation and break-up of large vortex structures was studied. An order of magnitude reduction in computational time is reported compared to direct numerical simulations is reported. Although an eight times smaller grid than a resolved DNS is used, the mean and r.m.s. velocity show very good agreement with the experimental results, see also Figure 8.14. It is argued that the under-resolved
Figure 8.11: Mean and r.m.s. velocity at the symmetry plane \( y = 0 \) for the turbulent flow around the Ahmed body, – KBC, ○ Experiment.
Figure 8.12: Mean velocity vectors \((u_y, u_z)/u_\infty\) at the slant and in the wake of the Ahmed body, − KBC, – Experiment.
8.5.3 Transitional Flows past Airfoil

In Dorschner et al. [187] simulations of transitional flows around airfoils were conducted using block grid-refinement. A detailed study on the flow around an SD7003 airfoil at Reynolds number $Re = 6 \cdot 10^4$ based on the chord length $c$ and uniform inflow velocity, and an angle of attack $\alpha = 4^\circ$ is carried out and compared to experiments and LES simulations. A domain of size $10c \times 5c \times 0.2c$ is chosen with $c = 1600$ lattice units at the highest refinement which results in a spatial resolution of $\Delta y^+ \approx 2.1$ at the wall. Figure 8.15 shows the comparison
Chapter 8  Complex and Wall-bounded turbulent Flows

(a) Geometry of the piston-valve assembly and illustration of vortex ring formation (pressure iso-surface and velocity magnitude).

(b) Mean and r.m.s. velocity profiles; comparison to DNS [185] and experiment [186].

Figure 8.14: Instantaneous vortex ring formation and multi-cycle averaged mean and r.m.s. velocity profiles in a engine-like piston valve assembly at 90° crank angle. Source: Dorschner et al. [117].

of the mean pressure coefficient along the surface. An investigation of the laminar separation bubble characteristics resulted in a very good agreement with experiments and LES simulations. It is pointed out here as well, that excellent agreement with reference data was achieved for all simulations despite the significantly coarser computational mesh compared to a fully refined DNS [187].
Chapter 8 Complex and Wall-bounded turbulent Flows

(a) Vorticity isosurfaces colored by streamwise velocity. (b) Average pressure coefficient $C_p$ over the upper and lower surface of the airfoil; comparison to LES simulations of Galbraith et al. [188] and Zhou et al. [189].

Figure 8.15: Transitional Flow around the SD8003 airfoil at Reynolds number $Re = 6 \cdot 10^4$ and angle of attack $\alpha = 4^\circ$. Source: Dorschner et al. [187].

8.6 Conclusions

The KBC models were tested for some complex and turbulent flows relevant for engineering applications. In particular, the flows considered here involve flat and curved walls and high Reynolds numbers. While almost all of the simulations presented here are not fully resolved, accurate predictions could be made with respect to the low-order velocity statistics, such as mean and r.m.s. fluctuations. All the KBC models run seamlessly without stability problems, while the standard LBGK model cannot be applied to such coarse resolutions. In case of the Flow around the Ahmed body previous attempts with LB had to resort to explicit turbulence modelling [179] while the parameter-free KBC models achieve good results and work "out of the box" for all the flows considered here and elsewhere [117, 134].

These results are encouraging the use of the parameter-free KBC models as drop-in replacement for engineering problems replacing explicit turbulence modelling. This is further substantiated by the favourable computational features of LB: efficiency, easily parallelizable and simple handling of complex geometries, to which the KBC models add only a small overhead in order to compute the entropic stabilizer.
Chapter 9

Extensions

The KBC was also extended to include more physics beyond the incompressible flow cases presented above. In particular, weakly compressible flows with temperature variations and two-phase flows with vapour-liquid interfaces are briefly presented below. The KBC models are added on top of established LB models. While the former case requires no modification of the KBC treatment, the latter case shows the incorporation of a force term. Furthermore, a novel LB method is developed for a binary mixture of two miscible components. Unlike previous attempts, the present mixture model provides an interpolation-free two-fluid approach with independent selection of viscosity and diffusivity. The KBC technique is extended for the quasi-equilibrium collision and two-dimensional benchmarks are presented.

9.1 Thermal Flows

In Pareschi et al. [190] the two-population model [29, 191, 192] for thermal flows at variable Prandtl numbers for standard lattices was extended to incorporate conjugate heat transfer between fluid and solids. In the two-population model a second lattice with coinciding nodes is introduced which is populated by distribution functions $g_i$ such that the post-collision states are defined by

$$f_i' = (1 - \beta) f_i + \beta f_i^\text{mirr}, \quad (9.1)$$
$$g_i' = (1 - \beta) g_i + \beta g_i^\text{mirr}, \quad (9.2)$$
with corresponding mirror states

\[ f_i^{\text{mirr}} = \frac{\omega}{\beta} f_i^{\text{eq}} - f_i + \left(2 - \frac{\omega}{\beta}\right) f_i^*, \quad (9.3) \]

\[ g_i^{\text{mirr}} = \frac{\omega}{\beta} g_i^{\text{eq}} - g_i + \left(2 - \frac{\omega}{\beta}\right) g_i^*, \quad (9.4) \]

where \( f_i^* \) and \( g_i^* \) denote the quasi-equilibrium distribution functions [191] and the relaxation parameters \( \beta \) and \( \omega \) control the viscous dissipation and the thermal diffusion, respectively. The set of local equilibrium constraints is extended in order to guarantee total energy conservation and thus enabling temperature dynamics,

\[ \rho = \sum_i f_i = \sum_i f_i^{\text{eq}}, \quad (9.5) \]

\[ \rho u_\alpha = \sum_i v_i^\alpha f_i = \sum_i v_i^\alpha f_i^{\text{eq}}, \quad (9.6) \]

\[ 2\rho E = 2\rho c_v T + \rho u_\alpha u_\alpha = \sum_i g_i = \sum_i g_i^{\text{eq}}, \quad (9.7) \]

with mass density \( \rho \), momentum \( \rho u_\alpha \), energy density \( E \), temperature \( T \) and heat capacity at constant volume \( c_v \). The two lattices \( f \) and \( g \) are one-way and locally coupled, that is to say, the hydrodynamic variables \( \rho \) and \( u_\alpha \) computed in \( f \) are used by the second lattice \( g \) but there is no feed-back of the temperature to the momentum equation. This results in a slightly corrupted momentum and energy equations which are however still valid for uncompressed thermal flows [29].

In order to recover the correct temperature dynamics and hydrodynamics the low order equilibrium moments for the fluid must be chosen as follows [29, 190],

\[ q_{\alpha}^{\text{eq},f} = \sum_i v_i^\alpha g_i^{\text{eq},f} = 2\rho E_f u_\alpha + 2\rho T_0 u_\alpha, \quad (9.8) \]

\[ R_{\alpha\beta}^{\text{eq},f} = \sum_i v_i^\alpha v_i^\beta g_i^{\text{eq},f} = 2\rho E_f (T_0 \delta_{\alpha\beta} + u_\alpha u_\beta) + 2\rho T_0 (T_0 \delta_{\alpha\beta} + 2u_\alpha u_\beta), \quad (9.9) \]

\[ S_{\alpha\beta\gamma}^{\text{eq},f} = \sum_i v_i^\alpha v_i^\beta v_i^\gamma g_i^{\text{eq},f} = 2\rho T_0 (E_f + 2T_0) (u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta}), \quad (9.10) \]

with the fluid energy density \( E_f = DT/2 + \rho u_\alpha u_\alpha/2 \) (note that \( c_v^f = D/2 \) fixed), reference temperature \( T_0 = 1/3 \) and \( P_{\alpha\beta}^{\text{eq}} \) and \( Q_{\alpha\beta\gamma}^{\text{eq}} \) as in the standard isothermal case given in Eqs. (2.10), (2.11).
The equilibrium moments for the solid regions on the other hand are [190],

\[ q_{eq,s}^a = \sum_i v_i g_i^{eq,s} = 0, \]  
\[ R_{eq,s}^{a\beta} = \sum_i v_i v_i \beta g_i^{eq,s} = 2 \rho_s T_0 (E_s + T_0) \delta_{a\beta}, \]  
\[ S_{eq,s}^{a\beta\gamma} = \sum_i v_i v_i \beta v_i \gamma g_i^{eq,s} = 0, \]  

with solid energy density \( E_s = c_s^v T \) (\( c_s^v \) is the heat capacity of the solid) and solid density \( \rho_s = 1 \).

The requirements on the quasi-equilibrium for the fluid are given as follows [190, 191],

\[ \sum_i g_i^{*,f} = 2 \rho E_f, \]  
\[ \sum_i v_i a g_i^{*,f} = q_a - 2 u_\beta \left( P_a^{f} - P_{eq,a}^{f} \right), \]  
\[ \sum_i v_i a v_i \beta g_i^{*,f} = R_{eq,s}^{a\beta}. \]  

Note that in the solid region, the kinetic equations for \( f \)-populations are not solved and no quasi-equilibrium \( g_{*,s} \) is required, and thus we can set \( \omega = 2 \beta \) in the solid region in Eq. 9.4. On the other hand, the quasi-equilibrium in the fluid region, \( f^* \), can be chosen as

\[ f^* = f_{eq}, \]  

for Prandtl numbers \( Pr \leq 1 \) [190]. In this case, Equation (9.3) reduces to the common incompressible case (2.4) and the thermal diffusivity of the fluid and solid are given by

\[ \alpha_f = \frac{k_f}{\rho c_f^v} = T_0 \left( \frac{1}{\omega_f} - \frac{1}{2} \right), \]  
\[ \alpha_s = \frac{k_s}{\rho_s c_s^v} = T_0 \left( \frac{1}{\omega_s} - \frac{1}{2} \right), \]  

with thermal conductivities \( k_f, k_s \) for the fluid and solid, respectively. The viscosity of the fluid is still determined by \( \beta \) through Eq. (2.14) and thus the Prandtl number is given by

\[ Pr = \frac{\nu}{\alpha_f} = \frac{(2-\beta) \omega_f}{(2-\omega_f) \beta}, \]  

In order to evaluate equilibrium and quasi-equilibrium states, the Grad’s approximation [113] (see also Eq. (5.60)) is used which can be written in the following generic form

$$ f_i^{\text{Grad}} = W_i \left( M_0 + \frac{M_\alpha v_{i\alpha}}{T_0} + \frac{(M_{\alpha\beta} - M_0 T_0 \delta_{\alpha\beta})(v_{i\alpha} v_{i\beta} - T_0 \delta_{\alpha\beta})}{2 T_0^2} \right) $$

(9.21)

for a scalar moment $M_0$, first-order moment $M_\alpha$ and second-order moment $M_{\alpha\beta}$. Upon substitution of $T_0 = 1/3$, $M_0 = \rho$, $M_\alpha = \rho u_\alpha$ and $M_{\alpha\beta} = P^{\text{eq}}_{\alpha\beta}$ the polynomial equilibrium (2.13) is recovered identically. The quasi-equilibrium $g^{*,f}$ and equilibria $g^{\text{eq},f}$, $g^{\text{eq},s}$ are computed in a similar manner, see also [190] for details.

The kinetic equations for the $f$ lattice are equivalent to the previously considered incompressible case and thus the KBC technique is readily applied to (9.1) using the model KBC-N2. Note, that the second lattice is not subject to any entropic stabilization and Eq. 9.2 is used as is.

Finally, the conjugate heat transfer between solid and fluid is realized by appropriate boundary conditions which ensure temperature continuity in wall normal direction as well as normal heat-flux continuity [190].

(a) Top: Numerical setup; Bottom: Instantaneous temperature distribution in the epoxy layer (b) Temperature profiles (symbols) along three selected lines and comparison to LES simulation [193].

**Figure 9.1:** Conjugate heat transfer in the turbulent flow over a wall-mounted matrix of cubes at $Re = 3854$. Source: Pareschi et al. [190].
A three-dimensional benchmark simulation is carried out in [190] where an array of surface mounted cubes with a hot core and an enveloping conducting epoxy layer submersed in a turbulent flow is analysed. The flow is characterized by Prandtl number $\text{Pr} = 0.712$, Reynolds number $\text{Re} = 3854$, based on the mean bulk velocity and cube height $h = 100$, and a thermal conductivity ratio of $k_2/k_1 = 9.183$ (with heat capacity ratio $c_2/c_1 = 10$) is used. The computational domain has dimensions $4h \times 4h \times 3.4h$ using adiabatic walls. Periodic boundary conditions are applied for the momentum equation, however, the temperature field uses inflow at fixed temperature and outflow boundary conditions. Results have been compared to experiment and simulations. Figure 9.1 shows the numerical setup, instantaneous temperature distribution and temperature profiles along three selected lines. Accurate results are reported while the KBC model contributes to the reliability and stability of the proposed model [190].

### 9.2 Two-Phase Flows

Two-phase flows are of fundamental interest in science and engineering applications [194]. Multi-phase flows expose a number of complex phenomena such as surface tension effects, droplet breakup and reconnection and liquid-wall interaction which are challenging for numerical methods [10]. The lattice Boltzmann method is considered as an attractive alternative to conventional methods based on the continuum equations or molecular dynamics and many LB variations have been proposed, see e.g. the reviews in [6, 52, 195]. In particular, the interface between liquid and vapour is realized by intermolecular forces which supersedes the explicit interface tracking required in other methods. Two popular classes of LB models for two-phase flows are the pseudo-potential methods originally proposed by Shan et al. [196] and the free-energy based methods by Swift et al. [9]. The latter methods offer a thermodynamically consistent approach in contrast to the former. However, the early two-phase LB models could not achieve sufficiently high density ratios and were prone to numerical instabilities [10]. The entropic free-energy based formulation of Mazloomi M et al. [10] on the other hand uses ELBM in connection with an optimal choice for the equation of state. Here we follow this approach and reformulate the method for the KBC models. The free-energy formulation requires the adherence to the Korteweg stress
Chapter 9 Extensions

tensor \[\text{[197]},\]

\[P_{\alpha\beta}^K = \left( p - \kappa \rho \partial_\gamma \partial_\gamma \rho - \frac{\kappa}{2} (\partial_\gamma \rho)(\partial_\gamma \rho) \right) \delta_{\alpha\beta} + \kappa (\partial_\alpha \rho)(\partial_\beta \rho), \quad (9.22)\]

where the pressure \(p\) is prescribed through a non-ideal equation of state and \(\kappa\) controls the surface tension. In order to incorporate the above Korteweg stress tensor in the LB formulation one can either modify the equilibrium accordingly (pressure approach) or introduce the effects dictated by the stress through a body force (forcing approach). The latter method is preferably followed in [10] because of better numerical stability.

The force acting on the liquid-vapour interface is thus given by

\[F_\alpha = \partial_\beta \left( \rho c_s^2 \delta_{\alpha\beta} - P_{\alpha\beta}^K \right), \quad (9.23)\]

where the first term is a correction to eliminate the pressure gradient stemming from the ideal equation of state inherent to the LB method (2.9).

Upon substitution of Eq. (9.22) in (9.23) the force term can be rearranged,

\[F_\alpha = 2 \varphi \partial_\alpha \varphi - \kappa \rho \partial_\alpha \left( \partial_\beta \partial_\beta \rho \right), \quad (9.24)\]

with

\[\varphi = \sqrt{\rho c_s^2 - p}. \quad (9.25)\]

The formulation (9.24) is particularly suitable from a practical viewpoint. The differential operators are subsequently discretized, which leads to

\[F_\alpha = 2 \varphi \overline{D}_\alpha \varphi - \kappa \rho \overline{D}_\alpha L \rho, \quad (9.26)\]

where \(D_\alpha\) and \(L\) are second-order finite difference (FD) approximations of the gradient and Laplace operator, respectively. In order to prevent non-physical shapes due to large spurious velocities, the gradient stencils are spatially window-averaged, see also [198],

\[\overline{D}_x \left|_{(x,y,z)} \right. = \sum_{j=-1}^{1} \sum_{k=-1}^{1} w_j w_k D_{x \left|_{(x,y+j,z+k)} \right.} \quad (9.27)\]

with weights \(w_0 = \frac{2}{3}, w_{\pm1} = \frac{1}{6}\) as exemplary shown here for the \(x\)-gradient.

Finally, the body force is applied through the exact difference method [137], see also Equation (8.7), with velocity increment

\[\Delta u_\alpha = \frac{F_\alpha}{\rho \Delta t}, \quad (9.28)\]
and $\Delta t = 1$. Hence, the LB equation can be written as

$$f_i(x + v_i, t + 1) = f_i' \equiv (1 - \beta) f_i(x, t) + \beta f_i^{\text{mirr}}(x, t) + F_i(x, t),$$

(9.29)

with

$$F_i = f_i^{\text{eq}}(\rho, u + \Delta u) - f_i^{\text{eq}}(\rho, u).$$

(9.30)

The KBC methodology can be extended to incorporate the force term (9.30) and an estimate for the entropic stabilizer is given by

$$\gamma = \frac{1}{\beta} + \left(1 - \frac{1}{\beta}ight) \frac{\langle \Delta s \mid \Delta h \rangle'}{\langle \Delta h \mid \Delta h \rangle'},$$

(9.31)

with the shifted entropic scalar product

$$\langle X \mid Y \rangle' = \sum_i X_i Y_i \frac{f_i^{\text{eq}}(\rho, u + \Delta u)}{f_i^{\text{eq}}(\rho, u + \Delta u)}.$$  

(9.32)

The equation of state chosen here is a polynomial regularization of the Peng-Robinson form [199] introduced in [10] and given by

$$p = 5.3 \cdot 10^{-2} \rho - 3.818183621928911 \cdot 10^{-2} \rho^2 + 4.139745482116095 \cdot 10^{-3} \rho^3$$

$$+ 3.748484095210317 \cdot 10^{-4} \rho^4 - 1.4552652965531227 \cdot 10^{-4} \rho^5$$

$$+ 1.2746947442749278 \cdot 10^{-5} \rho^6,$$

(9.33)

which amounts to a density contrast of $\rho_v / \rho_l \approx 100$ with liquid and vapour densities $\rho_l \approx 7.55$ and $\rho_v \approx 0.073$, respectively.

The surface tension $\sigma$ can be adjusted independently from the viscosity and grid size through the parameter $\kappa$. This is tested through confirmation of Laplace’s law

$$\Delta p = \sigma R,$$

(9.34)

where $\Delta p$ is the pressure difference between the liquid in the center of a droplet and the vapour pressure far away from the interface. Figure 9.2 shows the variation of the pressure difference with droplet radius $R$ for different values of $\kappa$ and kinematic viscosity $\nu = 0.05$. It is evident that the above two-phase KBC model adheres to Equation (9.34) and the corresponding values for the surface tension $\sigma$ can be computed from the slope of the lines. Moreover, the results coincide precisely with the values computed through the LBGK model without the KBC step. Independence of viscosity has been confirmed
**Figure 9.2:** Confirmation of Laplace’s Law with KBC and LBGK for various values of the surface tension parameter $\kappa$, where the surface tension $\sigma$ increases with increasing $\kappa$.

by repeating the same numerical experiment for different viscosities, $\nu = 0.1$, $\nu = 0.02$.

Using the surface tension estimated from Fig 9.2 a three-dimensional simulation of a droplet collision was chosen as benchmark, because droplet collisions involve a number of complex phenomena which are challenging from a computational viewpoint [201]. The two droplets undergo a head-on collision which results in eventual separation. The droplets have a size ratio of $R_l/R_s = 1.5$ with the smaller radius $R_s = 50$ lattice units and $\kappa = 0.002$ ($\sigma = 0.287$). The collision Weber number is defined by $We = 2\rho_l R_s U^2 / \sigma = 52.8$, with relative impact velocity $U$, and Reynolds number is $Re = 2R_s U / \nu = 245$.

We compare the result with the experiments of Tang et al. [200] who used tetradecane droplets with sizes of $R_s \approx 100 \mu m$. Figure 9.3 shows the evolution with time for the simulation and the experimental photographic images. The agreement in the droplet shapes and the temporal matching is predicted with good accuracy. It must be noted, that this simulation is not possible with the bare model using the LBGK collision model due to numerical instabilities. The KBC stabilization is acting foremost on the interface between the liquid and vapour phases but also inside the liquid perhaps triggered by large localized pressure. This behaviour is also illustrated in Figure 9.4.
Figure 9.3: Comparison of droplet shapes with experimental results [200] (top) and KBC simulation (bottom) for a binary head-on collision of two unequal sized droplets at Weber number $\text{We} = 52.8$.

Figure 9.4: Top: instantaneous spatial density distribution; Bottom: instantaneous spatial distribution of the stabilizer $\gamma$. Departure from LBGK value $\gamma = 2$ is visible mainly at the liquid-vapour interface.


9.3 Binary Mixtures

The subject of binary and multi-component mixtures has received considerable attention in the LB literature, see e.g. [12, 196, 202–230]. Modelling diffusion effects of the miscible species was attempted by various means, where earlier models were either based on simple passive scalar models or were directly derived from continuous (BGK type) kinetic models involving pseudo-potential interactions and heuristic free energy models. For more details the reader is referred to reviews [215, 216] and references therein. A brief overview of more recent LB models for mixtures is given below.

One can broadly distinguish between the single fluid approach using one lattice with pseudo-potential interactions (see e.g. [196]) or long-range coupling forces to model the cross collisions between different species and the two-fluid approach where a dedicated lattice is used for each species. The former approach entails a dependence between viscosity and diffusivity, and either of them cannot be chosen independently as well as a dependence of the mixture velocity on the relaxation time [216]. The two-fluid approach, on the other hand, has no such limitation and the coupling can be realized by force term in the momentum equation [216], however, it is considered computationally more expensive [227].

Arcidiacono et al. [218] introduced a thermodynamically consistent genuine lattice Boltzmann two-fluid model based on the quasi-equilibrium model [191, 231], which satisfies the indifferentiability principle, which states that the two-species equations reduce to the single-fluid equations for identical components [232]. The model is able to handle arbitrary mass ratios of the two species, and the speed of sound of the species $s$ is given by

$$c_s = \sqrt{\frac{kT}{m_s}}, \quad (9.35)$$

with Boltzmann constant $k$, temperature $T$ and the molecular mass $m_s$ of species $s$. In order to account for the difference in the speed of sound between the different species, the grids spanned by the lattices are scaled accordingly. This results in non-coinciding grid nodes and requires spatial interpolation. The viscosity can be chosen independently from the diffusivity, which is characterized by the Stefan-Maxwell diffusion equation. This model was then refined in [219] to include two different quasi-equilibrium states, which are selected adaptively based on entropic considerations. The two relaxation
regimes are differentiated by the Schmidt number,

$$Sc = \frac{\mu}{\rho D_{AB}},$$

(9.36)

where $\mu$ denotes the dynamic viscosity, $\rho$ is the mixture density and $D_{AB}$ is the binary diffusion coefficient of the species $A$ and $B$. Subsequently, this model was extended to multiple species using the mixture averaged diffusion approximation [220] and has been applied to simulate reacting flows where realistic mixture transport coefficients were obtained through coupling to the Chemkin package. Asinari [224, 225] used a single-fluid MRT model for low Mach number flows based on the model by Andries et al. [232] for multiple components which does not resort to the mixture-average diffusion approximation but relies on non-local terms evaluated with finite differences. Shan [227] proposed a single-fluid model based on a direct discretization of the BGK-type continuous Boltzmann equation using non-local interactions based on a pseudo-potential approach. The importance of adhering to the energy equipartition principle was pointed out, which states that the particles of each species should have the same averaged kinetic energy in the reference frame moving with the barycentric mixture velocity

$$u = \frac{j}{\rho},$$

(9.37)

with mixture momentum $j = \sum_s j_s = \sum_s \rho_s u_s$, and mixture density $\rho = \sum_s \rho_s$ at thermal equilibrium. In other words, the internal kinetic energy is related to the temperature $T$ by

$$2\rho E_{\text{int}} = 2\rho E - \rho u_a u_a = D n k T,$$

(9.38)

with total energy $\rho E = \sum_s \rho_s E_s$, dimension $D$ and mixture number density $n = \sum_s n_s$, which implies that heavier particles have smaller averaged thermal speed [227], see also Eq. (9.35). According to [227], this was not explicitly satisfied in the earlier athermal multicomponent LB models which likely led to deviations from Graham’s law. Kang et al. [228] developed a two-fluid thermal model for binary mixtures based on the single component thermal model on standard lattices [233] and make use of non-local counter terms to correct for the low symmetry of the standard lattices together with quasi-equilibrium similar approach as [218, 219]. The same model was later extended to support multiple components [229]. Tong et al. [230] improved the two-fluid multi-component model [223] with independent viscosities and diffusivities, and
thus avoiding the mixture averaged approximation, where the diffusion is dictated by the Stefan-Maxwell model. The lattices are scaled according to the molecular weight of the species and the collision involves a BGK term to account for self-collisions and a second term for the cross-collisions between different components.

Here we follow the two-fluid approach and in particular we adopt the quasi-equilibrium model [218], however, the inclusion of energy conservation allows the fulfilment of the energy equipartition principle and a similar equilibrium as in [227] is used. Moreover, the two lattices for the binary mixture have coinciding nodes and thus the need for spatial interpolation is eliminated. The speed of sound is modelled correctly and the pressure is given by the ideal gas equation of state

\[ p = nkT. \]  

(9.39)

The following model was developed in collaboration with the Master student Felix Thaler.

### 9.3.1 Model Description

The discrete kinetic equations for a binary mixture can be written as

\[
\begin{align*}
    f_{si}(x + v_{si}\Delta t, t + \Delta t) &= f'_{si}(x, t) \equiv (1 - \beta)f_{si}(x, t) + \beta f_{si}^{\text{mirr}}(x, t), \\
    f_{si}^{\text{mirr}}(x, t) &= \omega \beta f_{si}^{\text{eq}}(x, t) - f_{si}(x, t) + \left(2 - \frac{\omega}{\beta}\right)f_{si}^{*}(x, t),
\end{align*}
\]

(9.40)

with the discrete velocity vector \(v_{si}\), substance index \(s = A, B\) and \(i = 1, \cdots, N_s\). Similar to the previous models by Arcidiacono et al. [218–220], the present model belongs to the class of quasi-equilibrium kinetic models [191]. \(f_{si}^{\text{eq}}\) and \(f_{si}^{*}\) are the equilibrium and quasi-equilibrium distribution functions (populations), respectively, and the relaxation parameters \(\beta\) and \(\omega\) control the viscous dissipation of the mixture and the binary diffusion of the components. The populations \(f_{si}\) are carried on two lattices with coinciding nodes, corresponding to the components \(A\) and \(B\) of the mixture, which reduces implementation complexity, prevents additional numerical diffusion and increases computational efficiency.
The pertinent moments for the populations \( f_s \) are defined as

\[
\sum_i f_{si} = n_s \\
m_s \sum_i f_{si} = \rho_s \\
m_s \sum_i f_{si} v_{sia} = j_{sa} \\
m_s \sum_i f_{si} v_{sia} v_{sia} = 2 \rho_s E_s \\
m_s \sum_i f_{si} v_{sia} v_{sip} = P_{sa\beta} \\
m_s \sum_i f_{si} v_{sia} v_{sip} v_{sip} = q_{sa} \\
m_s \sum_i f_{si} v_{sia} v_{sip} v_{siy} = Q_{sa\beta\gamma} \\
m_s \sum_i f_{si} v_{sia} v_{sip} v_{siy} v_{siy} = R_{sa\beta},
\]

with number density \( n_s \), mass density \( \rho_s = n_s m_s \), mass flux \( j_{sa} = \rho_s u_{sa} \), total energy \( 2\rho_s E_s \), symmetric pressure tensor \( P_{sa\beta} \), heat flux \( q_{sa} \), and the symmetric third order moment \( Q_{sa\beta\gamma} \) as well as the once contracted fourth order moment \( R_{sa\beta} \).

The moments for populations \( f_s^* \) and \( f_s^{\text{eq}} \) are defined analogously and denoted with superscript \((\cdot)^*\) and \((\cdot)^{\text{eq}}\), respectively, and the local conservation laws of mass, momentum and energy imply

\[
n_s = n_s^* = n_s^{\text{eq}}, \quad \rho_s = \rho_s^* = \rho_s^{\text{eq}}, \quad j = \sum_s j_s = \sum_s j_s^* = \sum_s j_s^{\text{eq}} = \rho u, \\
2\rho E = \sum_s 2\rho_s E_s = \sum_s 2\rho_s E_s^* = \sum_s 2\rho_s E_s^{\text{eq}} = DnkT + \rho u_a u_\alpha,
\]

where the barycentric equilibrium momentum and the equilibrium energy are defined as

\[
j_s^{\text{eq}} = Y_s j, \quad \rho_s E_s^{\text{eq}} = DX_s nkT + X_s \rho u_a u_\alpha.
\]

using definitions for mole and mass fractions, \( X_s = n_s / n \) and \( Y_s = \rho_s / \rho \), respectively. The mass flux and energy for species \( s \) are given by the quasi-
equilibrium moments, can be written as a linear combination,

$$j_s^* = (1 - \varphi) j_s + \varphi j_{s}^{eq},$$  \hspace{1cm} (9.48)

$$E_s^* = (1 - \varphi) E_s + \varphi E_{s}^{eq},$$  \hspace{1cm} (9.49)

according to (9.44) and (9.45) with the parameter $\varphi$ to be determined.

The equilibrium and quasi-equilibrium populations can be found as minimizers of the discrete H-function

$$H = \sum_s \sum_i f_{si} \ln \frac{f_{si}}{W_{si}},$$  \hspace{1cm} (9.50)

subject to relevant constraints, where $W_{si}$ are the lattice weights. The constraints for the equilibrium are composed of local conservation of (number) density, mixture momentum and mixture energy given by equations (9.42) - (9.45). The quasi-equilibrium additionally locally conserves the substance mass flux and substance energy and thus the relevant constraints are given by equations (9.43), (9.48) and (9.49). The choice of the conserved variables and quasi-conserved variables only differs from the previous models [218–220] in the additional conservation of energy. Indeed, this change is the key to capture the correct speed of sound in the mixture on a single grid and to satisfy the equipartition principle.

In order to respect the correct temperature dynamics thermal multi-speed lattices as proposed in [30] are used here. These lattices can capture the correct speed of sound in a (limited) range of temperatures and mass ratios. In particular, the positivity range at zero velocity for the thermal $D2Q25$ lattice is given by

$$\frac{1}{3} < \frac{kT}{m_s} < 3$$ \hspace{1cm} (9.51)

and thus the upper bound for the mass ratio is

$$\frac{m_B}{m_A} = 9$$ \hspace{1cm} (9.52)

in the case of constant temperature and in general, $\frac{m_B}{m_A} < 9 \frac{T_{min}}{T_{max}}$, assuming $m_A \leq m_B$.

Note that in most LB models the particle (molecular) mass is assumed to be unity. When the substances involved have different molecular masses $m_s$, the corresponding speed of sound may only be respected by stretching the lattice for the heavier substance. In contrast to previous approaches, the present
model avoids this scaling. Thus, the lattices coincide which allows for a local scheme without interpolation which reduces implementation complexity and prevents numerical diffusion.

The solution of the minimization problem (9.50) can be directly inferred from the solution for a single component fluid \[218\] and recovers the pertinent Maxwell-Boltzmann moments until fourth order in velocity for the \(D2Q25\) lattice \[30, 101\]. The single component solution leads to the formal solution, 

\[
f^P_i(n, u, \theta) = n W_i \exp \left[ \chi'_a v_{ia} + \zeta'_a v_{ia} \phi v_{ia} \right] \tag{9.53}
\]

with temperature dependent weights \(W_i(\theta)\) and Lagrange multipliers \(\chi'(u, \theta), \zeta'_a(u, \theta)\) and \(\phi'(u, \theta)\) to be determined upon substitution into the constraints, which can be reformulated as the particularly efficient product form,

\[
f^P_i(n, u, \theta) = n W_i \chi_{\alpha}^i v_{\alpha}^i \phi v_{\alpha}^i, \tag{9.54}
\]

where the Lagrange multipliers can be evaluated using a power-series expansion in velocity \(u_\alpha\), for low Mach number flows. The weights on the other hand are determined by matching to the lower even-order Maxwell-Boltzmann moments at zero velocity. For further details and explicit expressions for the weights and the Lagrange multipliers the reader is referred to Frapolli et al. \[30\].

Finally, the equilibrium and quasi-equilibrium can be computed using the product form (9.54),

\[
f_{si}^{eq} = f^P_{si}(n_s, u, kT/m_s), \tag{9.55}
\]

\[
f_{si}^{*} = f^P_{si}(n_s, u^*, kT/m_s), \tag{9.56}
\]

\[
f_{si} = f^P_{si}(n_s, j^*, kT/m_s), \tag{9.57}
\]

with the quasi-equilibrium quantities

\[
u^* = j^*/\rho_s, \tag{9.58}
\]

\[
2 \rho_s E^* = D n_s kT^*_s + \rho_s u^*_{sa} u^*_{sa}. \tag{9.59}
\]

For the equilibrium moments we thus have \[30\]

\[
P_{s\alpha\beta}^{eq} = n_s kT \delta_{\alpha\beta} + \rho_s u_\alpha u_\beta + O(u^4, u^2 \Delta V^2, \Delta V^4), \tag{9.60}
\]

\[
Q_{s\alpha\beta\gamma}^{eq} = n_s kT (u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta}) + \rho_s u_\alpha u_\beta u_\gamma 
+ O(u^5, u^3 \Delta V^2, u \Delta V^4), \tag{9.61}
\]

\[
R_{s\alpha\beta}^{eq} = n_s kT ((D + 2) kT/m_s + u_\gamma u_\gamma) \delta_{\alpha\beta} + (D + 4) n_s kT u_\alpha u_\beta 
+ O(u^4, u^2 \Delta V^2, \Delta V^4), \tag{9.62}
\]
with the lattice sound speed deviation \( \Delta V_s = \sqrt{kT/m_s} - \sqrt{v_0^2} \) and \( v_0^2 = 0.36754 \) and similar expressions are obtained for the quasi-equilibrium moments.

### 9.3.2 Derivation of Transport Coefficients

The relaxation parameters \( \beta \) and \( \omega \) as well as the parameter \( \phi \) are determined by the Chapman-Enskog method and related to the transport coefficients. To this end, Equation (9.40) is rewritten,

\[
f_{sl}(x + v_{sl}\delta t, t + \delta t) - f_{sl}(x, t) = 2 \beta (f^*_s(x, t) - f_{sl}(x, t)) + \omega (f^\text{eq}_s(x, t) - f^*_s(x, t)),
\]

and the left hand side of equation (9.63) is expanded using a Taylor series to second order

\[
\left[ \delta t (\partial_t + \partial_a v_{sia}) + \frac{\delta t^2}{2} (\partial_t + \partial_a v_{sia}) (\partial_t + \partial_\beta v_{si\beta}) \right] f_{si} = 2 \beta (f^*_s - f_{si}) + \omega (f^\text{eq}_s - f^*_s).
\]

By introducing a characteristic time scale of the flow, \( \Theta \), we can rewrite (9.64) in a non-dimensional form using reduced variables \( t' = t/\Theta, v'_{si} = v_{si}/c \) and \( x' = x/(v\Theta) \), where \( v = 1 \). After introduction of the parameter \( \epsilon = \delta t/\Theta \) and dropping the primes to simplify notation we get

\[
\left[ \epsilon (\partial_t + \partial_a v_{sia}) + \frac{\epsilon^2}{2} (\partial_t + \partial_a v_{sia}) (\partial_t + \partial_\beta v_{si\beta}) \right] f_{si} = 2 \beta (f^*_s - f_{si}) + \omega (f^\text{eq}_s - f^*_s).
\]

By exploiting the smallness of \( \epsilon \) we can perform a multi-scale expansion of the time derivative operator and the populations until second order,

\[
\epsilon \partial_t = \epsilon \partial_t^{(1)} + \epsilon^2 \partial_t^{(2)} + \cdots \tag{9.66}
\]

\[
f_{si} = f_{si}^{(0)} + \epsilon f_{si}^{(1)} + \epsilon^2 f_{si}^{(2)} + \cdots \tag{9.67}
\]

\[
f^*_s = f^*_s^{(0)} + \epsilon f^*_s^{(1)} + \epsilon^2 f^*_s^{(2)} + \cdots. \tag{9.68}
\]

Inserting (9.66) - (9.68) into eq. (9.65) we can analyze the terms corresponding to orders \( \epsilon^0 \), \( \epsilon^1 \) and \( \epsilon^2 \). The zeroth order terms lead to

\[
0 = 2 \beta (f^*_s - f_{si}^{(0)}) + \omega (f^\text{eq}_s - f^*_s^{(0)}), \tag{9.69}
\]

which implies

\[
f_{si}^{(0)} = f^*_s^{(0)} = f^\text{eq}_s. \tag{9.70}
\]
Local conservation laws dictate the following solvability conditions for the higher order terms ($p > 0$)

\begin{align*}
  n_s^{(p)} &= \sum_i f_s^{(p)} = 0, \\
  n_s^{*(p)} &= \sum_i f_s^{*(p)} = 0, \\
  j_a^{(p)} &= \sum_s m_s \sum_i f_s^{(p)} v_{sia} = 0, \\
  j_a^{*(p)} &= \sum_s m_s \sum_i f_s^{*(p)} v_{sia} = 0, \\
  2\rho E^{(p)} &= \sum_s m_s \sum_i f_s^{(p)} v_{sia} v_{sia} = 0, \\
  2\rho E^{*(p)} &= \sum_s m_s \sum_i f_s^{*(p)} v_{sia} v_{sia} = 0,
\end{align*}

and

\begin{align*}
  j_s^{(p)} &= \frac{1}{1 - \phi} j_s^{*(p)}, \\
  E_s^{(p)} &= \frac{1}{1 - \phi} E_s^{*(p)}.
\end{align*}

The terms of order $\epsilon^1$ lead to

\begin{align*}
  (\partial_t^{(1)} + \partial_a v_{sia}) f_{si}^{eq} &= -2\beta f_{si}^{(1)} + (2\beta - \omega) f_{si}^{*(1)},
\end{align*}

from which we can recover the thermo-hydrodynamic equations of mass, momentum and energy to first order by taking the zeroth, first and second order moment of (5.33). Using solvability conditions and definitions of $P_{a\beta}^{eq} = \sum_s P_{sa\beta}^{eq}$ and $q_a^{eq} = \sum_s q_{sa}^{eq}$ we get for the substance $s$

\begin{align*}
  \partial_t^{(1)} n_s + \partial_a \left( X_s \frac{j_a}{m} \right) &= 0, \\
  \partial_t^{(1)} \rho_s + \partial_a (Y_s j_a) &= 0, \\
  \partial_t^{(1)} (Y_s j_a) + \partial_a p_s + \partial_p \left( Y_s \frac{j_a j_b}{\rho} \right) &= \left( \frac{2\phi \beta + (1 - \phi) \omega}{\phi - 1} \right) j_{sa}^{*(1)}, \\
  \partial_t^{(1)} (2\rho_s E_s^{eq}) + \partial_a \left( (D + 2)p_s \frac{j_a}{\rho} + Y_s \frac{j_a j_b j_b}{\rho^2} \right) &= \left( \frac{2\phi \beta + (1 - \phi) \omega}{\phi - 1} \right) 2\rho_s E_s^{*(1)},
\end{align*}
with partial pressure \( p_s = X_s p = X_s n k T \). For the mixture we have

\[
\begin{align*}
\partial_t^{(1)} n + \partial_{\alpha}(nu_{\alpha}) &= 0, \\
\partial_t^{(1)} \rho + \partial_{\alpha}(\rho u_{\alpha}) &= 0, \\
\partial_t^{(1)} u_{\alpha} + u_{\beta}\partial_{\beta} u_{\alpha} + \frac{1}{\rho}\partial_{\alpha} p &= 0, \\
\partial_t^{(1)} T + u_{\alpha}\partial_{\alpha} T + \frac{2}{D} T \partial_{\alpha} u_{\alpha} &= 0.
\end{align*}
\]

By evaluating the time derivative in eq. (9.82) and (9.83) using Eqs. (9.81), (9.85), (9.86) and (9.87) we get

\[
\begin{align*}
p\left( (X_s - Y_s) \frac{\partial_{\alpha} p}{p} + \partial_{\alpha} X_s \right) &= \left( \frac{2\varphi \beta + (1 - \varphi)\omega}{\varphi - 1} \right) j_{\alpha}^{*(1)} s, \\
p j_{\alpha} \left( (X_s - Y_s) \frac{\partial_{\alpha} p}{p} + \partial_{\alpha} X_s \right) &= \left( \frac{2\varphi \beta + (1 - \varphi)\omega}{\varphi - 1} \right) \rho_{s} E_{s}^{*(1)}.
\end{align*}
\]

Collecting terms of order \( \epsilon^2 \) results in

\[
\begin{align*}
\left[ \partial_t^{(2)} + \left( \partial_t^{(1)} + \partial_{\alpha} v_{\alpha} \right) \left( \frac{1}{2} - \frac{1}{2\beta} \right) \left( \partial_{\alpha}^{(1)} + \partial_{\alpha} v_{\alpha} \right) \right] f_{si}^{eq} \\
+ \left( \partial_t^{(1)} + \partial_{\alpha} v_{\alpha} \right) \left( \frac{2\beta - \omega}{2\beta} \right) f_{si}^{*(1)} = -2\beta f_{si}^{(2)} + (2\beta - \omega) f_{si}^{*(2)}.
\end{align*}
\]

Thus, the second order equation for the substance density yields

\[
\partial_t^{(2)} \rho_{s} + \partial_{\alpha} \left[ \left( \frac{1}{2} - \frac{1}{2\beta} \right) \left( \frac{2\varphi \beta + (\varphi - 1)\omega}{\varphi - 1} \right) + \left( \frac{2\beta - \omega}{2\beta} \right) \right] j_{\alpha}^{*(1)} = 0.
\]

Let us now introduce the diffusion flux defined as

\[
V_{\alpha} = \rho_r \left( \frac{j_{\alpha}^{*a}}{\rho_A} - \frac{j_{\alpha}^{*b}}{\rho_B} \right),
\]

with reduced density \( \rho_r = \rho_A \rho_B / (\rho_A + \rho_B) \). Then, one can write

\[
\begin{align*}
j_{\alpha}^{*a} &= Y_{A} j_{\alpha} + V_{\alpha}, \\
j_{\alpha}^{*b} &= Y_{B} j_{\alpha} - V_{\alpha},
\end{align*}
\]

and hence the parameter \( \varphi \) is determined by

\[
\varphi = \frac{\omega}{2 + \omega - 2\beta},
\]
so that the second order density equation (9.91) for substance $s$ simplifies to

\[ \partial_t^{(2)} \rho_s + \partial_\alpha \left( j_{sa}^{(1)} \right) = 0, \tag{9.96} \]

which results in

\[ \partial_t^{(2)} \rho = 0, \tag{9.97} \]

for the mixture density. Using definition (9.92), the result (9.95) and Eq. (9.88) we get to first order

\[ \partial_\alpha X_A = \frac{\omega}{1 - \beta} \frac{\rho_r}{P} \left( \frac{j_{Ba}^*}{\rho_B} - \frac{j_{Aa}^*}{\rho_A} \right) + \left( Y_A - X_A \right) \frac{\partial_\alpha p}{p}, \tag{9.98} \]

which is then compared to the Stefan-Maxwell diffusion relation,

\[ \partial_\alpha X_A = \frac{X_A X_B}{D_{AB}} \left( \frac{j_{Ba}^*}{\rho_B} - \frac{j_{Aa}^*}{\rho_A} \right) + \left( Y_A - X_A \right) \frac{\partial_\alpha p}{p}, \tag{9.99} \]

and thus we get

\[ D_{AB} = \frac{1 - \beta}{\omega} \frac{p X_A X_B}{\rho_r} \tag{9.100} \]

for the binary diffusion coefficient $D_{AB}$. The second order equation for the mixture momentum results is

\[ \partial_t^{(2)} \left( \rho u_\alpha \right) + \partial_\beta \left[ \left( \frac{1}{2} - \frac{1}{2\beta} \right) \left( \partial_t^{(1)} P_{\alpha\beta}^{eq} + \partial_\gamma Q_{\alpha\beta\gamma}^{eq} \right) + \frac{2\beta - \omega}{2\beta} P^{(1)}_{\alpha\beta} \right] = 0. \tag{9.101} \]

The quasi-equilibrium pressure tensor can be evaluated from its definition, and hence,

\[ P^{*}_{a\beta} = n_s k T^{*}_{s} \delta_{a\beta} + \frac{j_a j_{s\beta}^{*}}{\rho} + \frac{j_{Aa} j_{sa}^{*}}{\rho} \]

\[ = \frac{1}{D} \left[ 2 \rho_s E_{s}^{*} - \frac{2 j_{sy}^{*}}{\rho} j_{y} \right] \delta_{a\beta} + \frac{j_a j_{s\beta}^{*}}{\rho} + \frac{j_{Aa} j_{sa}^{*}}{\rho}, \tag{9.102} \]

\[ P^{*}_{a\beta} = 0. \tag{9.103} \]

By evaluating the spatial gradients in Eq. (9.101) and using the first order results (9.84)-(9.86), the second order equation for the mixture velocity results in

\[ \partial_t^{(2)} u_\alpha + \frac{1}{\rho} \Pi_{a\beta} = 0, \tag{9.104} \]
with the non-equilibrium pressure tensor $\Pi_{\alpha\beta}$ and rate of strain tensor $S_{\alpha\beta}$

$$\Pi_{\alpha\beta} = -\mu \left( S_{\alpha\beta} - \frac{2}{D} \partial_\gamma u_\gamma \delta_{\alpha\beta} \right),$$

(9.105)

$$S_{\alpha\beta} = \partial_\beta u_\alpha + \partial_\alpha u_\beta,$$

(9.106)

and thus the viscosity is identified by

$$\nu = \frac{\mu}{\rho} = \frac{p}{\rho} \left( \frac{1}{2\beta} - \frac{1}{2} \right).$$

(9.107)

### 9.3.3 Entropic Stabilization

For increased numerical stability, the KBC procedure is applied to the quasi-equilibrium kinetic model. The mirror state is partitioned by

$$f_{si}^{\text{mirr}} = k_i + 2s_{si}^{\text{eq,G}} - s_{si} + \gamma h_{si}^{\text{eq,G}} + (1 - \gamma) h_{si},$$

(9.108)

with the generalized equilibrium

$$f_{si}^{\text{eq,G}} = \frac{\omega'}{\beta} f_{si}^{\text{eq}} + \left( 1 - \frac{\omega'}{\beta} \right) f_{si}^*,$$

(9.109)

and

$$2\omega' = \omega.$$

(9.110)

The kinematic part $k_{si}$ depends only on the locally conserved density, $s_{si}$ depends on the momentum and shear moments (i.e. stress tensor) and $h_{si}$ on the remaining higher order moments. The estimate for the entropic stabilizer $\gamma$ is then computed analogously to Eq. (5.6).

### 9.3.4 Speed of Sound

The speed of sound in a mixture is $c_s = \sqrt{\gamma k_B T / m}$, where $\gamma$ is the adiabatic exponent, and $m = \sum_s X_s m_s$ is the mixture molecular mass. The speed of sound was measured in a two-dimensional shock tube simulation with spatially constant molar fraction. The $D2Q25 - ZOT$ lattice with base velocities $v_{1a} = \{0, \pm 1, \pm 3\}$ was employed. Note that the enhanced isotropy of the multi-speed lattice is needed to capture the correct speed of sound if $m_A \neq m_B$. Only in cases where the molecular masses of both species are identical, standard lattices can be used as well. Figure 9.5 shows the speed of sound measured by the present model for a range of molar fractions $X_A$, and compared to theoretical results. The simulation demonstrates that the present model correctly captures the non-linear behaviour of the mixture speed of sound.
Figure 9.5: Speed of sound in a binary mixture. Measurements were obtained from a 2D shock tube simulation. The circles and continuous line show the measured and theoretical results, respectively. A molar mass ratio of $m_B/m_A = 4$ was used.

### 9.3.5 Binary Diffusion

For the simple initial condition of zero velocity and a molar fraction with step profile, analytical solutions exist for the binary diffusion. The present initial condition is

\[
X_A = X_0, \quad X_B = 1 - X_0, \quad \text{if } x < 0, \\
X_A = 1 - X_0, \quad X_B = X_0, \quad \text{if } x \geq 0. \tag{9.111}
\]

The parameter $X_0$ defines the initial molar fractions. The analytical solution is [219, 234]

\[
X_A = \frac{1}{2} - \frac{X_0 - \frac{1}{2}}{2} \text{erf} \left( \frac{x}{\sqrt{4D_{AB}t}} \right). \tag{9.112}
\]

Figure 9.6 shows results for different Schmidt numbers, compared to the analytical solutions, with excellent agreement.

The effect of the proposed entropic stabilization is illustrated in Figure 9.7 where a comparison of an unstabilized ($\gamma = 2$) and stabilized diffusion simulation with low viscosity is shown. The stabilized version clearly prevents the large oscillations which lead to numerical problems which eventually lead to a catastrophic failure.
Figure 9.6: Binary diffusion started with initial condition given in Eq. (9.111). Shown is the molar fraction of component A at time $t = 1000$ for different Schmidt numbers: $Sc = 0.1$ (circles), $Sc = 1$ (squares) and $Sc = 10$ (diamonds). The kinematic viscosity is $\nu = 0.2$, the mass ratio $m_B/m_A = 4$. The continuous lines show the analytical solutions.

### 9.3.6 Rayleigh-Taylor Instability

To validate the model in a more dynamic scenario, we chose the Rayleigh-Taylor instability (RTI) as a test case and compared the initial exponential growth to the results from linear stability theory (LST). The classical RTI considers two fluids on top of each other, the upper with density $\rho_U$ being heavier than the lower with density $\rho_L$. The LST allows to predict an initial exponential growth of a small perturbation

$$\eta(t) = \eta_0 e^{\phi t}$$  \hspace{1cm} (9.113)

on the interface, where $\phi$ is the exponential growth coefficient and $\eta_0$ is the initial amplitude. Assuming inviscid flow and no diffusion, $\phi$ depends on the Atwood number

$$A = (\rho_U - \rho_L)/(\rho_U + \rho_L),$$  \hspace{1cm} (9.114)

gravitational acceleration $g$ and wave-number $k$ of the disturbance only, namely $\phi = \sqrt{Agk}$. For the viscid and miscible case Duff et al. [235] proposed the more accurate approximation

$$\phi = \sqrt{Agk/\psi + \nu^2 k^4} - (\nu + D_{AB}) k^2,$$  \hspace{1cm} (9.115)
Figure 9.7: Binary diffusion with $Sc = 1$, $m_B/m_A = 2$ and $\nu = 10^{-3}$. The simulation with entropic stabilization (continuous line) is stable at the initial discontinuity while the unstabilized solver (dashed line) is not.

where the function $\psi$ accounts for dynamic diffusion. Following Taylor [236] we choose the initial perturbation and velocity field to be

$$\eta_0 = Bk \cos(kx)/\phi,$$  \hspace{1cm} (9.116)

where $B$ is a small constant, combined with the initial velocity field

$$u_0 = \begin{cases} 
-Be^{-ky} \sin kx, -Be^{-ky} \cos kx & \text{if } y \geq 0, \\
Be^{ky} \sin kx, -Be^{ky} \cos kx & \text{if } y < 0.
\end{cases}$$ \hspace{1cm} (9.117)

For reasons of stability, the initial molar fraction field was slightly smoothed. The measured amplitudes compared to LST results are depicted in Figure 9.8. A constant value of $\psi$ was fitted to the measurements. Exact quantitative comparison to LST is difficult for the given case, especially as we observed relatively large effects of the initial diffusion on $\psi$. Still, our results clearly show exponential growth in the correct order of magnitude, with increasing coefficient $\phi$ for larger Schmidt numbers. The slight deviation between observed growth and LST at late times is expected due to emerging non-linear effects.

Three snapshots of the molar fraction are depicted in Figure 9.9, showing the typical dynamics of the RTI after the initial exponential growth phase. As the
Figure 9.8: Exponential growth of a small single-mode perturbation in the RTI. For the simulation, we chose $A = 0.243$, $m_B / m_A = 2$, $g = 0.0002$, $\nu = 0.05$, $\rho_L = X m_A + (1 - X) m_B$ and $\rho_U = (1 - X) m_A + X m_B$ with $X = 0.865$. The symbols show our results for $Sc = 0.2$ (circles), $Sc = 1$ (squares) and $Sc = 100$ (diamonds). The continuous lines show LST results with the growth coefficient from Eq. (9.115) and fitted constant $\psi$. The dashed line is the inviscid and immiscible LST result.

Schmidt number here is $Sc = 10$, the diffusion of the interface is relatively weak compared to the convective effects and the interface stays sharp for a relatively long time.

9.4 Conclusions

The applicability and universal character of the KBC models is demonstrated for three different fluid dynamical regimes beyond the single component incompressible flows. Adoption of KBC stabilization in the two-population thermal model is straight-forward as only the lattice carrying the momentum is altered. The three-dimensional simulation of the flow around an array of heated surface mounted cubes demonstrates the usefulness of the KBC model for thermal flows. The second extension shows the application of KBC to a hydrodynamic system with a non-ideal equation of state. The liquid-vapour interface is established by adopting Korteweg’s stress tensor through an external force, and hence, the KBC formulas are slightly altered to accommodate for this additional source term. The three-dimensional simulation of a droplet
collision shows the effectiveness of KBC, where it allows for a substantial Weber number at a large density contrast. The original two-phase model used here as point or origin became possible in the first place by employing the entropic LB method (ELBM), and hence, we show that with the KBC a similar stabilization effect can be achieved in this case.

The multi-speed two-fluid binary mixture model developed in the third part in this chapter is new considering a number of aspects. It simultaneously satisfies the indifferentiability and energy equipartition principle, and uses the thermal multi-speed lattice D2Q25 to achieve non-unity mass ratios without scaling of the underlying lattice. This makes this model particularly attractive as no interpolations are necessary in this genuine, fully local, LB model. The mixture viscosity and binary diffusion coefficient can be chosen independently and the Stefan-Maxwell diffusion is recovered in the hydrodynamic limit. An array of two-dimensional benchmarks are carried out which show the consistency with theory; In particular, the mixture speed of sound and the binary diffusion are tested and results show excellent agreement with reference solutions. Moreover, the KBC method is extended to quasi-equilibrium
collision models and the effect of damping spurious numerical oscillations is shown exemplarily. Finally, the initial stages of a Rayleigh-Taylor instability are numerically investigated and good agreement with theory is achieved for different Schmidt numbers.
Chapter 10

Conclusions

A new perspective on the direct simulation of low-dissipative hydrodynamic flows using advanced fluid-kinetic theory is proposed in this thesis. Entropy control, with its solid physical background, significantly extends the operation range of the lattice Boltzmann method, with only a minute computational overhead. No tunable parameters, considerably higher stability and ease in the implementation are the salient features of the new KBC lattice Boltzmann models. Based on these observations, these models are particularly attractive approaches to the emergent fluid-kinetic simulation of complex flows and fluids, ranging from turbulence, to multiphase flows, thermal flows, multi-component mixtures and beyond.

10.1 Limitations

The KBC models improve numerical stability greatly when compared to LBGK or MRT models so that very coarse simulations can be conducted. However, this does not imply that results of severely under-resolved simulations are necessarily accurate to the same degree and was also pointed out by [237] who found that the KBC models are "virtually indestructible". Careful and thorough grid convergence studies are still necessary and the sub-grid-features of the KBC models must be further studied in detail, be it numerically or analytically. The mirror state (5.3) implies a nominally constant viscosity to the level of accuracy of the expansion in the derivation in Section 5.5. However, as shown in numerical simulations in Chapters 6-8 the influence of higher order terms on the macroscopic viscosity is evident in the under-resolved cases through a secondary dissipation mechanism, which arguably, helps stabilize the simulation numerically but does not prevent quantitatively good results for first and
second order statistics.

In the entropic LB method (ELBM) the entropy is guaranteed to grow by convexity of the $H$-function if a solution to the isentropic condition exists. The KBC models, in contrast, do not provide such a strong guarantee. The search space for the entropy maximization is confined to the hyper-plane spanned by the $h$-part which might not allow local growth of entropy, see also Figure 5.1 for a graphical representation. One may intuitively argue that, the larger the search space the more likely it is to find a solution for $\gamma$ which locally increases entropy. This is indeed supported by the fact that the low symmetry lattices $D3Q15$ and $D3Q19$ turned out to be considerably less stable than the $D3Q27$ or the $D2Q9$ lattice in our simulations. Analogously, the search space shrinks when more moments are included in the $s$-part. It is for instance not recommended to include the third order moments in $s$ for the two-dimensional $D2Q9$ lattice as this leaves only one free moment, $A$, in $h$ and stability is significantly reduced. The approximate solution to the stabilizer $\gamma$ by the estimate (5.6) may additionally hinder the maximization. On the other hand, the maximization can also yield results which exhibit higher entropy values than possible with ELBM (as is the case in the illustration in Figure 5.1) and furthermore, the estimate $\gamma^*$ was was in excellent agreement with the analytical formula in our numerical experiments.

10.2 Future Work

In order to further substantiate the validity and suitability of the KBC models for turbulent flows the range of applications must be broadened and more benchmark cases are to be simulated, but in the light of the promising res-ults, predictive simulations of industrial and engineering problems may be envisaged already.

It is clear, that more analytical and numerical studies are needed to understand the sub-grid behaviour in order to more precisely pinpoint the effects of the higher order terms on coarse-grid simulations. In that regard, comparisons to state-of-the-art turbulence models and LES simulations would be beneficial to demonstrate the viability and advantages of the KBC approach. On the other hand, it may be of interest, as well, to use the entropic maximisation principle in order to find an optimal moment basis which orthogonally disentangles the higher order moments from the lower hydrodynamic moments in the sense of the entropic scalar product.
As the range of applications clearly goes beyond incompressible flows, interesting challenges in the realm of thermal flows should be targeted, such as convection phenomena in the Rayleigh-Bénard flow. In the same spirit, the multi-component mixture model should be extended to three dimensions with possible further developments to accommodate multiple components. Finally, a number of further extensions towards other physical mechanisms may be envisaged, with the magneto-hydrodynamics as an auspicious candidate, and in combination with turbulence, in particular.

The challenging regime of compressible flows has so far been resistive to the KBC treatment. On the other hand, the ELBM is the model of choice for the complex interplay between turbulence and shocks [31]. However, the discontinuities at the shock fronts may actually require an adaptive change in the viscosity itself, as is the case for DNS simulations of turbulence shock interactions, where a dissipative scheme is used in the vicinity of the shocks and a non-dissipative scheme is used to capture turbulence. On the other hand, the general KBC method employing multiple relaxation parameters, may be of help here to increase the search space for an optimal solution.

### 10.3 Results

Using the ideas borrowed from the entropic lattice Boltzmann method and the multiple relaxation time models, the KBC models are investigated in detail, and brought from academic examples, to canonical benchmarks, to isotropic homogeneous turbulence, and to complex flows involving relevant engineering scenarios. A particular focus was directed on the study of the performance of the parameter-free models in the case of under-resolved simulations. Apart from exceptional stability, the sub-grid scale features are promising and, due to the adaptive nature of the model, the scope of application is wide and has proven most general. Low-order statistics are captured with good accuracy even when the flow is severely under-resolved. On the other hand, the entropic stabilization entails a secondary implicit dissipation mechanism which takes control when stability is in danger due to the rise of sharp gradients which would otherwise quickly lead to a catastrophic outcome. Contrary to the gradients, the turbulence kinetic energy remains largely unaffected by this process. Moreover, the artificial dissipation was measured in simulations and found to be reasonably small even for coarse grids. Most importantly, the models recover the Navier-Stokes with the expected accuracy and shows the
Chapter 10  Conclusions

correct limit in a fully resolved case. Energy and enstrophy spectra as well as scaling laws indicate that the turbulence characteristics are captured with good accuracy. Comparison between presented simulations and experimental and numerical data for complex flows in turbulent settings provides compelling evidence of increased stability and good accuracy of the new model. Such simulations were hitherto hardly possible without the use of sub-grid turbulence models. 

The general nature of the KBC approach calls for applications and extensions beyond the incompressible low Mach number flows, and extensions towards thermal flows, two-phase flows and binary mixtures are presented. The seamless adoption of the KBC models to these physically different regimes contributes to the overall assessment and the universal character of the entropy maximisation. While the two-phase flow model, as well as the thermal model, pre-existed and were merely adapted to account for the KBC collision, a novel model for binary mixture was developed during this thesis. The salient features of the binary mixture model are the lack of interpolation and the use of thermal multi-speed lattices to account for the different sound speed of the two unequally heavy substances involved. The results are in very good agreement with the reference solutions. Independent adjustment of the diffusion coefficient and kinematic viscosity of the mixture is assured and the diffusion follows the Stefan-Maxwell model.

In summary, by exploiting the degrees of freedom of MRT and by approximate compliance to the $H$-theorem, the advantages of both methods are retained and the problems of parameter tuning and fluctuating viscosity are solved. The resulting family of KBC models are accurate, adaptive, parameter-free, efficient and, also supremely stable and may provide the long sought-after unification of the scattered field of different multi-relaxation models, enabling applications for turbulent flows and complex geometries and may also be readily generalized to different regimes of fluid dynamics and thus may potentially have a significant scientific impact.
Appendix

A.1 Central Moment Representation for D3Q27

The mapping between natural and central moments is linear in the non-conserved moments and given by the following relations:

\[ \tilde{P}_{xy} = P_{xy} - u_x u_y \]  \hspace{1cm} (A.1)

\[ \tilde{P}_{xz} = P_{xz} - u_x u_z \]  \hspace{1cm} (A.2)

\[ \tilde{P}_{yz} = P_{yz} - u_y u_z \]  \hspace{1cm} (A.3)

\[ \tilde{N}_{xz} = N_{xz} - u_x^2 + u_z^2 \]  \hspace{1cm} (A.4)

\[ \tilde{N}_{yz} = N_{yz} - u_y^2 + u_z^2 \]  \hspace{1cm} (A.5)

\[ \tilde{T} = T - (u_x^2 + u_y^2 + u_z^2) \]  \hspace{1cm} (A.6)

\[ \tilde{Q}_{xy} = Q_{xy} - u_x \tilde{P}_{yz} - u_y \tilde{P}_{xz} - u_z \tilde{P}_{xy} - u_x u_y u_z \]  \hspace{1cm} (A.7)

\[ \tilde{Q}_{xy} = Q_{xy} - \frac{1}{3} \left( 6 u_y \tilde{P}_{xy} + u_x (3 u_y^2 + 2 \tilde{N}_{yz} - \tilde{N}_{xz} + \tilde{T}) \right) \]  \hspace{1cm} (A.8)

\[ \tilde{Q}_{xz} = Q_{xz} - \frac{1}{3} \left( 6 u_z \tilde{P}_{xz} + u_x (3 u_z^2 - \tilde{N}_{xz} - \tilde{N}_{yz} + \tilde{T}) \right) \]  \hspace{1cm} (A.9)

\[ \tilde{Q}_{xy} = Q_{xy} - \frac{1}{3} \left( 6 u_x \tilde{P}_{xy} + u_y (3 u_x^2 + 2 \tilde{N}_{xz} - \tilde{N}_{yz} + \tilde{T}) \right) \]  \hspace{1cm} (A.10)
\[ \tilde{Q}_{yyz} = Q_{yyz} - \frac{1}{3} \left( 6u_y \tilde{P}_{yz} + u_y (3u_z^2 - \tilde{N}_{xz} - \tilde{N}_{yz} + \tilde{T}) \right) \]  (A.11)

\[ \tilde{Q}_{xxz} = Q_{xxz} - \frac{1}{3} \left( 6u_x \tilde{P}_{xz} + u_x (3u_y^2 + 2\tilde{N}_{xz} - \tilde{N}_{yz} + \tilde{T}) \right) \]  (A.12)

\[ \tilde{Q}_{yyz} = Q_{yyz} - \frac{1}{3} \left( 6u_y \tilde{P}_{yz} + u_y (3u_z^2 + 2\tilde{N}_{xz} - \tilde{N}_{yz} + \tilde{T}) \right) \]  (A.13)

\[ \tilde{M}_{022} = M_{022} - \left( u_z^2 u_x^2 + 4u_y u_z \tilde{P}_{yz} + (u_y^2 + u_z^2) \tilde{T}/3 - (u_y^2 + u_z^2) \tilde{N}_{xz}/3 \right. \\
+ \left. (-u_z^2 + 2u_y^2) \tilde{N}_{yz}/3 + 2u_y \tilde{Q}_{yyz} + 2u_z \tilde{Q}_{yyz} \right) \]  (A.14)

\[ \tilde{M}_{202} = M_{202} - \left( u_z^2 u_x^2 + 4u_x u_z \tilde{P}_{xz} + (u_x^2 + u_z^2) \tilde{T}/3 + (u_x^2 + 2u_z^2) \tilde{N}_{xz}/3 \right. \\
- \left. (u_x^2 + u_z^2) \tilde{N}_{yz}/3 + 2u_x \tilde{Q}_{zzz} + 2u_z \tilde{Q}_{zzz} \right) \]  (A.15)

\[ \tilde{M}_{220} = M_{220} - \left( u_z^2 u_y^2 + 4u_x u_y \tilde{P}_{xy} + (u_x^2 + u_y^2) \tilde{T}/3 + (-u_x^2 + 2u_y^2) \tilde{N}_{xz}/3 \right. \\
+ \left. (2u_x^2 - u_y^2) \tilde{N}_{yz}/3 + 2u_x \tilde{Q}_{xyz} + 2u_y \tilde{Q}_{xyz} \right) \]  (A.16)

\[ \tilde{M}_{211} = M_{211} - \left( u_x u_z u_y + 2u_x u_z \tilde{P}_{xy} + 2u_x u_y \tilde{P}_{xz} + u_x^2 \tilde{P}_{yz} + u_y u_z \tilde{T}/3 \right. \\
+ \left. 2u_y u_z \tilde{N}_{xz}/3 - u_y u_z \tilde{N}_{yz}/3 + 2u_x \tilde{Q}_{xxy} + u_z \tilde{Q}_{xyz} + u_y \tilde{Q}_{yyz} \right) \]  (A.17)

\[ \tilde{M}_{121} = M_{121} - \left( u_x u_z u_y + 2u_x u_y \tilde{P}_{zy} + u_y^2 \tilde{P}_{xz} + 2u_x u_y \tilde{P}_{yz} + u_x u_z \tilde{T}/3 \right. \\
- \left. u_x u_z \tilde{N}_{xz}/3 + 2u_x u_z \tilde{N}_{yz}/3 + 2u_y \tilde{Q}_{xyz} + u_z \tilde{Q}_{xyz} + u_x \tilde{Q}_{yyz} \right) \]  (A.18)

\[ \tilde{M}_{112} = M_{112} - \left( u_x u_y u_z^2 + u_z \tilde{P}_{xy} + 2u_y u_z \tilde{P}_{xz} + 2u_x u_y \tilde{P}_{yz} + u_x u_y \tilde{T}/3 \right. \\
- \left. u_x u_y \tilde{N}_{xz}/3 - u_x u_y \tilde{N}_{yz}/3 + 2u_z \tilde{Q}_{xyz} + u_y \tilde{Q}_{xyz} + u_x \tilde{Q}_{yyz} \right) \]  (A.19)

\[ \tilde{M}_{122} = M_{122} - \left( u_x u_y u_z^2 + 2u_y u_z^2 \tilde{P}_{xy} + 2u_y u_z \tilde{P}_{xz} + 4u_x u_y u_z \tilde{P}_{yz} \right. \\
+ (u_x u_y^2 + u_x u_z^2) \tilde{T}/3 + (u_x u_y^2 - u_x u_z^2) \tilde{N}_{xz}/3 \\
+ (u_x u_y^2 + u_x u_z^2) \tilde{N}_{yz}/3 + 4u_y u_z \tilde{Q}_{xyz} + u_z^2 \tilde{Q}_{xyz} + u_y^2 \tilde{Q}_{yyz} \\
+ 2u_x u_y \tilde{Q}_{yyz} + 2u_x u_z \tilde{Q}_{yyz} + 2u_y \tilde{M}_{112} + 2u_z \tilde{M}_{121} + u_x \tilde{M}_{022} \right) \]  (A.20)
\[
\tilde{M}_{212} = M_{212} - (u_x^2 u_y u_z^2 + 2u_x u_z^2 \tilde{P}_{xy} + 4u_x u_y u_z \tilde{P}_{xz} + 2u_x^2 u_z \tilde{P}_{yz} \\
+ (u_x^2 u_y + u_y u_z^2) \tilde{T}/3 + (-u_x^2 u_y + 2u_y u_z^2) \tilde{N}_{xz}/3 \\
+ (-u_x^2 u_y - u_y u_z^2) \tilde{N}_{yz}/3 + 4u_x u_y \tilde{Q}_{xyz} + 2u_x u_z \tilde{Q}_{xxy} + u_z^2 \tilde{Q}_{xyy} \\
+ u_x^2 \tilde{Q}_{yyz} + 2u_y u_z \tilde{Q}_{zzz} + 2u_z \tilde{M}_{211} + 2u_x \tilde{M}_{121} + u_y \tilde{M}_{202}) \tag{A.21}
\]

\[
\tilde{M}_{221} = M_{221} - (u_x^2 u_y u_z^2 + 4u_x u_y u_z \tilde{P}_{xy} + 2u_x u_y^2 \tilde{P}_{xz} + 2u_x^2 u_y \tilde{P}_{yz} \\
+ (u_x^2 u_y + u_y u_z^2) \tilde{T}/3 + (-u_x^2 u_y + 2u_y u_z^2) \tilde{N}_{xz}/3 \\
+ (2u_x^2 u_z - u_y u_z^2) \tilde{N}_{yz}/3 + 4u_x u_y \tilde{Q}_{xyz} + 2u_x u_z \tilde{Q}_{xxy} + 2u_y u_z \tilde{Q}_{xyy} \\
+ u_y^2 \tilde{Q}_{xxz} + u_x^2 \tilde{Q}_{yyz} + 2u_y \tilde{M}_{211} + 2u_x \tilde{M}_{121} + u_z \tilde{M}_{220}) \tag{A.22}
\]

\[
\tilde{M}_{222} = M_{222} - (u_x^2 u_y u_z^2 + 4u_x u_y u_z^2 \tilde{P}_{xy} + 4u_x u_y^2 u_z \tilde{P}_{xz} + 4u_x^2 u_y u_z \tilde{P}_{yz} \\
+ (u_x^2 u_y^2 + u_x^2 u_z^2 + u_y^2 u_z^2) \tilde{T}/3 + (-u_x^2 u_y^2 - u_x^2 u_z^2 + 2u_y^2 u_z^2) \tilde{N}_{xz}/3 \\
+ (-u_x^2 u_y^2 + 2u_x^2 u_z^2 - u_y^2 u_z^2) \tilde{N}_{yz}/3 + 8u_x u_y u_z \tilde{Q}_{xyz} + 2u_x u_z^2 \tilde{Q}_{xzy} \\
+ 2u_x u_y^2 \tilde{Q}_{xxz} + 2u_y u_z^2 \tilde{Q}_{yyz} + 2u_x^2 u_y \tilde{Q}_{yyz} + 2u_y^2 u_z \tilde{Q}_{xyy} \\
+ u_x^2 \tilde{M}_{022} + u_y^2 \tilde{M}_{202} + u_z^2 \tilde{M}_{220} + 4u_y u_z \tilde{M}_{211} + 4u_x u_z \tilde{M}_{121} \\
+ 4u_x u_y \tilde{M}_{112} + 2u_z \tilde{M}_{212} + 2u_y \tilde{M}_{212} + 2u_z \tilde{M}_{221}) \tag{A.23}
\]
Substituting Eqs. (A.1)-(A.23) in Eq. (2.41) one arrives at the moment representation in the central basis:

\[ f_{(0,0,0)} = \rho \left( - \left( u_x^2 - 1 \right) \left( u_y^2 - 1 \right) \left( u_z^2 - 1 \right) - 4 u_x u_y \left( u_z^2 - 1 \right) \tilde{P}_{xy} 
+ 4 u_x u_z \left( u_y^2 - 1 \right) \tilde{P}_{xz} - 4 u_y u_z \left( u_x^2 - 1 \right) \tilde{P}_{yz} 
+ \left( u_x^2 \left( u_y^2 + u_z^2 - 2 \right) + u_y^2 \left( 1 - 2 u_x^2 \right) + u_z^2 \right) \tilde{N}_{xz} / 3 
+ \left( u_y^2 \left( u_x^2 + u_z^2 - 2 \right) + u_z^2 \left( 1 - 2 u_y^2 \right) + u_x^2 \right) \tilde{N}_{yz} / 3 
- \left( u_x^2 u_y^2 + u_y^2 u_z^2 + u_z^2 u_x^2 - 2 \left( u_x^2 + u_y^2 + u_z^2 \right) + 3 \right) \tilde{T} / 3 
- 8 u_x u_y u_z \tilde{Q}_{xyz} - 2 u_x \left( u_z^2 - 1 \right) \tilde{Q}_{xyy} - 2 u_x \left( u_y^2 - 1 \right) \tilde{Q}_{xzz} 
- 2 u_y \left( u_z^2 - 1 \right) \tilde{Q}_{xxz} - 2 u_y \left( u_x^2 - 1 \right) \tilde{Q}_{yyz} - 2 u_y \left( u_y^2 - 1 \right) \tilde{Q}_{zzx} 
- 2 u_z \left( u_x^2 - 1 \right) \tilde{Q}_{xyy} + \left( 1 - u_x^2 \right) \tilde{M}_{022} + \left( 1 - u_y^2 \right) \tilde{M}_{202} + \left( 1 - u_z^2 \right) \tilde{M}_{220} 
- 4 u_y u_z \tilde{M}_{211} - 4 u_x u_z \tilde{M}_{121} - 4 u_x u_y \tilde{M}_{112} - 2 u_x \tilde{M}_{122} - 2 u_y \tilde{M}_{112} 
- 2 u_z \tilde{M}_{221} - \tilde{M}_{222} \right) \]  

(A.24)

\[ f_{(\sigma,0,0)} = \frac{1}{\rho} \rho \left( 3 u_x \left( u_y^2 - 1 \right) \left( u_z^2 - 1 \right) \left( \sigma + u_x \right) + 6 u_y \left( u_z^2 - 1 \right) \left( \sigma + u_x \right) \tilde{P}_{xy} 
+ 6 u_z \left( u_y^2 - 1 \right) \left( \sigma + 2 u_x \right) \tilde{P}_{xz} + 12 u_x u_y u_z \left( \sigma + u_x \right) \tilde{P}_{yz} 
- \left( \sigma u_x \left( u_y^2 + u_z^2 - 2 \right) + u_x \left( u_y^2 + u_z^2 - 2 \right) - 2 \left( u_y^2 - 1 \right) \left( u_z^2 - 1 \right) \right) \tilde{N}_{xz} 
+ \left( u_z^2 \left( 2 u_x \left( \sigma + u_x \right) - u_y^2 \right) + u_x \left( u_y^2 + 1 \right) \left( \sigma + u_x \right) + u_z^2 \right) \tilde{N}_{yz} 
+ \left( u_x^2 \left( u_x \left( \sigma + u_x \right) + u_y^2 \right) + u_x \left( u_y^2 - 2 \right) \left( \sigma + u_x \right) - u_y^2 - u_z^2 + 1 \right) \tilde{T} 
+ 12 u_x u_y \left( \sigma + 2 u_x \right) \tilde{Q}_{xyz} + 3 \left( u_y^2 - 1 \right) \left( \sigma + 2 u_x \right) \tilde{Q}_{xyy} 
+ 3 \left( u_y^2 - 1 \right) \left( \sigma + 2 u_x \right) \tilde{Q}_{xzz} + 6 u_y \left( u_z^2 - 1 \right) \tilde{Q}_{xyy} + 6 u_x u_y \left( \sigma + u_x \right) \tilde{Q}_{yyz} 
+ 6 u_y \left( u_y^2 - 1 \right) \tilde{Q}_{xzz} + 6 u_x u_y \left( \sigma + u_x \right) \tilde{Q}_{yyz} + 3 u_x \left( \sigma + u_x \right) \tilde{M}_{022} 
+ 3 \left( u_y^2 - 1 \right) \tilde{M}_{202} + 3 \left( u_z^2 - 1 \right) \tilde{M}_{220} + 12 u_y u_z \tilde{M}_{211} 
+ 6 u_x u_y \left( \sigma + 2 u_x \right) \tilde{M}_{121} + 6 u_y \left( \sigma + 2 u_x \right) \tilde{M}_{112} 
+ 3 \left( \sigma + 2 u_x \right) \tilde{M}_{122} + 6 u_y \tilde{M}_{212} + 6 u_x \tilde{M}_{221} + 3 \tilde{M}_{222} \right) \]  

(A.25)
\begin{align}
\begin{aligned}
    f_{(0,\lambda,0)} &= \frac{1}{6} \rho \left[ 3u_y (u_x^2 - 1) (u_y^2 - 1) (\lambda + u_y) + 6u_x (u_x^2 - 1) (\lambda + 2u_y) \tilde{P}_{xy} \\
    &+ 12u_x u_y u_z (\lambda + u_y) \tilde{P}_{xz} + 6u_z (u_x^2 - 1) (\lambda + 2u_y) \tilde{P}_{yz} \\
    &+ (-u_x^2 (u_y (\lambda + u_y) + u_z - 1) + u_y (2u_x^2 - 1) (\lambda + u_y) + u_z^2 - 1) \tilde{N}_{xz} \\
    &+ (-u_x^2 (u_y (\lambda + u_y) - 2u_z^2 + 2) - u_y (u_z^2 - 2) (\lambda + u_y) - 2u_z^2 + 2) \tilde{N}_{yz} \\
    &+ (u_x^2 (u_y (\lambda + u_y) + u_z^2 - 1) + u_y (u_z^2 - 2) (\lambda + u_y) - u_z^2 + 1) \tilde{T} \\
    &+ 12u_x u_y u_z (\lambda + 2u_y) \tilde{Q}_{xyz} + 6u_x (u_z^2 - 1) \tilde{Q}_{xyy} + 6u_y u_y (\lambda + u_y) \tilde{Q}_{xyy} \\
    &+ 3(u_x^2 - 1) (\lambda + 2u_y) \tilde{Q}_{xyz} + 3(u_x^2 - 1) (\lambda + 2u_y) \tilde{Q}_{yyz} \\
    &+ 6u_y u_z (\lambda + u_y) \tilde{Q}_{xyz} + 6u_z (u_x^2 - 1) \tilde{Q}_{yyz} \right] + 3(u_x^2 - 1) (\lambda + 2u_y) \tilde{M}_{122} + 3 (\lambda + 2u_y) \tilde{M}_{121} + 6u_x (\lambda + 2u_y) \tilde{M}_{112} \\
    &+ 6u_x \tilde{M}_{122} + 3 (\lambda + 2u_y) \tilde{M}_{212} + 6u_x \tilde{M}_{221} + 3 \tilde{M}_{222} \\
\end{aligned}
\end{align}

(A.26)
\( f(\sigma, \lambda, 0) = \frac{1}{4} \rho \left( -u_x u_y (u_y^2 - 1)(\lambda + u_y)(\sigma + u_x) - (u_y^2 - 1)(\lambda + 2u_y)(\sigma + 2u_x)\hat{P}_{xy} - 2u_y u_z (\lambda + u_y)(\sigma + 2u_x)\hat{P}_{xz} - u_x u_z (\lambda + 2u_y)(\sigma + u_x)\hat{P}_{yz} \right. \\
\quad + \frac{1}{3} (\sigma u_x (u_y (\lambda + u_y) + u_y^2 - 1)) + u_x^2 (u_y(\lambda + u_y) + u_y^2 - 1) \\
\quad - 2u_y (u_y^2 - 1)(\lambda + u_y))\tilde{N}_{xz} + \frac{2}{3} (\sigma u_x (u_y (\lambda + u_y) - 2u_y^2 + 2)) \\
\quad + u_x^2 (u_y(\lambda + u_y) - 2u_y^2 + 2) + u_y (u_y^2 - 1)(\lambda + u_y))\tilde{N}_{yz} \\
\quad + \frac{1}{3} (-\sigma u_x (u_y (\lambda + u_y) + u_y^2 - 1) - u_x^2 (u_y(\lambda + u_y) + u_y^2 - 1) \\
\quad - u_y (u_y^2 - 1)(\lambda + u_y))\tilde{T} - 2u_z (\lambda + 2u_y)(\sigma + 2u_x)\tilde{Q}_{xyz} \\
\quad - (u_y^2 - 1)(\sigma + 2u_x)\tilde{Q}_{xyy} - u_y(\lambda + u_y)(\sigma + 2u_x)\tilde{Q}_{xzz} \\
\quad - (u_y^2 - 1)(\lambda + 2u_y)\tilde{Q}_{xxz} - u_x (\lambda + 2u_y)(\sigma + u_x)\tilde{M}_{022} \\
\quad - u_y (\lambda + u_y)\tilde{M}_{202} + \left(1 - u_y^2\right)\tilde{M}_{220} - 2u_z (\lambda + 2u_y)\tilde{M}_{211} \\
\quad - 2u_z (\sigma + 2u_x)\tilde{M}_{121} - (\lambda + 2u_y)(\sigma + 2u_x)\tilde{M}_{112} - (\sigma + 2u_x)\tilde{M}_{122} \\
\quad - (\lambda + 2u_y)\tilde{M}_{122} - 2u_z \tilde{M}_{221} - \tilde{M}_{222}) \\
\quad (A.28) \\
\end{array} \]

\( f(\sigma, 0, \delta) = \frac{1}{4} \rho \left( -u_x u_z (u_z^2 - 1)(\delta + u_z)(\sigma + u_x) - 2u_y u_z (\delta + u_z)(\sigma + 2u_x)\hat{P}_{xy} \\
\quad - \left( u_z^2 - 1 \right)(\delta + 2u_z)(\sigma + 2u_x)\hat{P}_{xz} - 2u_y u_z (\delta + 2u_z)(\sigma + u_x)\hat{P}_{yz} \\
\quad + \frac{1}{3} \left( \sigma u_x \left( u_z (\delta + u_z) + u_z^2 - 1 \right) + u_x^2 \left( u_z (\delta + u_z) + u_z^2 - 1 \right) \right) \\
\quad - 2 \left( u_z^2 - 1 \right) u_z (\delta + u_z))\tilde{N}_{xz} + \frac{2}{3} \left( \sigma u_x \left( -2u_z (\delta + u_z) + u_z^2 - 1 \right) \right) \\
\quad + u_x^2 \left( -2u_z (\delta + u_z) + u_z^2 - 1 \right) + \left( u_z^2 - 1 \right) u_z (\delta + u_z))\tilde{N}_{yz} \\
\quad + \frac{1}{3} \left( -\sigma u_x \left( u_z (\delta + u_z) + u_z^2 - 1 \right) - u_x^2 \left( u_z (\delta + u_z) + u_z^2 - 1 \right) \right) \\
\quad - \left( u_z^2 - 1 \right) u_z (\delta + u_z))\tilde{T} - 2u_y (\delta + 2u_z)(\sigma + 2u_x)\tilde{Q}_{xyz} \\
\quad - u_z (\delta + u_z)(\sigma + 2u_x)\tilde{Q}_{xyy} - \left( u_y^2 - 1 \right)(\sigma + 2u_x)\tilde{Q}_{xzz} - 2u_y u_z (\delta + u_z)\tilde{Q}_{xyz} \\
\quad - 2u_x u_y (\sigma + u_x)\tilde{Q}_{yzz} - \left( u_y^2 - 1 \right)(\delta + 2u_z)\tilde{Q}_{xxz} - u_x (\delta + 2u_z)(\sigma + u_x)\tilde{Q}_{yzz} \\
\quad - u_x (\sigma + u_x)\tilde{M}_{022} + \left(1 - u_y^2\right)\tilde{M}_{202} - u_z (\delta + u_z)\tilde{M}_{220} - 2u_y (\delta + 2u_z)\tilde{M}_{211} \\
\quad - (\delta + 2u_z)(\sigma + 2u_x)\tilde{M}_{121} - 2u_y (\sigma + 2u_x)\tilde{M}_{112} - (\sigma + 2u_x)\tilde{M}_{122} \\
\quad - 2u_y \tilde{M}_{212} - (\delta + 2u_z)\tilde{M}_{221} - \tilde{M}_{222}) \\
\quad (A.29) \)
\[ f(0, \lambda, \delta) = \frac{1}{4} \rho \left( -u_1 u_2 (u_2^2 - 1) (\delta + u_1 z) (\lambda + u_y) - 2u_1 u_2 (\delta + u_2 z) (\lambda + 2u_y) \tilde{P}_{xy} - 2u_1 u_2 (\delta + 2u_2 z) (\lambda + u_y) \tilde{P}_{xz} - (u_2^2 - 1) (\delta + 2u_2 z) (\lambda + 2u_y) \tilde{P}_{yz} \right. \\
+ \frac{1}{3} \left( \lambda u_y (u_2 (\delta + u_2 z) + u_2^2 - 1) + u_2^2 (u_2 (\delta + u_2 z) + u_2^2 - 1) \right) \\
+ \left. (u_2^2 - 1) u_2 (\delta + u_2 z) \right) \tilde{P}_{xz} + \frac{1}{3} \left( \lambda u_y (u_2 (\delta + u_2 z) + u_2^2 - 1) \right) \\
+ u_2^2 (u_2 (\delta + u_2 z) + u_2^2 - 1) - 2(u_2^2 - 1) u_2 (\delta + u_2 z) \right) \tilde{P}_{yz} \\
+ \frac{1}{3} \left( -\lambda u_y (u_2 (\delta + u_2 z) + u_2^2 - 1) - u_2^2 (u_2 (\delta + u_2 z) + u_2^2 - 1) \right) \\
- \left( u_2^2 - 1 \right) u_2 (\delta + u_2 z) \tilde{T} - 2u_2 (\delta + 2u_2 z) (\lambda + 2u_y) \tilde{Q}_{xyz} \\
- 2u_2 u_2 (\delta + u_2 z) \tilde{Q}_{xyy} - 2u_2 u_2 (\lambda + u_y) \tilde{Q}_{xzz} \\
- u_2 (\delta + u_2 z) (\lambda + 2u_y) \tilde{Q}_{xxy} - (u_2^2 - 1) (\lambda + 2u_y) \tilde{Q}_{yzz} \\
- u_2 (\delta + 2u_2 z) (\lambda + u_y) \tilde{Q}_{xxz} - (u_2^2 - 1) (\delta + 2u_2 z) \tilde{Q}_{yyz} + \left( 1 - u_2^2 \right) \tilde{M}_{022} \\
- u_2 (\lambda + u_y) \tilde{M}_{202} - u_2 (\delta + u_2 z) \tilde{M}_{220} - (\delta + 2u_2 z) (\lambda + 2u_y) \tilde{M}_{211} \\
- 2u_2 (\delta + 2u_2 z) \tilde{M}_{121} - 2u_2 (\lambda + 2u_y) \tilde{M}_{112} - 2u_2 \tilde{M}_{122} \\
- (\lambda + 2u_y) \tilde{M}_{121} - (\delta + 2u_2 z) \tilde{M}_{221} - \tilde{M}_{222} \right) \\
\text{(A.30)} \]
List of Tables

2.1 Discrete velocities and corresponding weights for the two standard lattices in two and three dimensions. ............................................. 15

5.1 Nomenclature key for the KBC models family for central and natural moments. For each model the moments constituting the $s$-part of the populations $f_i = k_i + s_i + h_i$ are indicated, where $Q$ consists of the moments $Q_{xzz}$, $Q_{xxy}$, $Q_{yyz}$, $Q_{xxz}$, $Q_{yy}$ and $Q_{xyz}$ (and analogously for the central moment $\tilde{Q}$). ............................................. 49

5.2 Second order moments for functions $s$ and $h$ in KBC A-D. .... 53

7.1 Characteristics for two-dimensional turbulence simulations (lattice units). .......................................................... 72

7.2 Comparison of LBGK and KBC-N4 for statistical quantities in Kida vortex flow at $Re = \frac{U_0 N}{\nu} = 6000$ and $t = \frac{N}{U_0} = 0.25, 0.5, 0.75$. Resolutions $N = 100, 200, 400, 600$ for KBC runs A, B, C and resolved LBGK run D, respectively. Convergence rate $p$ of error w.r.t. LBGK solution estimated from polynomial fit ($\ast$ indicates exclusion of lowest resolution). All gradient-based quantities are computed by spectral differentiation methods [130]. Turbulence characteristics: length scale $l_0 = k^{3/2}/\epsilon$, velocity scale $u_0 = k^{1/2}$, time scale $\tau_0 = l_0/u_0$, and Reynolds number $Re_0 = l_0 u_0/\nu$. Taylor characteristics: Taylor micro scale $\lambda = \left(15\nu u'^2/\epsilon\right)^{1/2}$, velocity scale $u_\lambda = u' = (2k/3)^{1/2}$ (r.m.s. turbulence intensity), time scale $\tau_\lambda = \lambda/u_\lambda$ and Reynolds number $Re_\lambda = \lambda u_\lambda/\nu$. Kolmogorov characteristics: length scale $\eta = (\nu^3/\epsilon)^{1/4}$, velocity scale $u_\eta = (\nu e)^{1/4}$ and time scale $\tau_\eta = (\nu/e)^{1/4}$. ............................................. 83

7.3 Relative difference in percentage of statistical quantities in Kida vortex flow at $Re = \frac{U_0 N}{\nu} = 6000$ for times $t = \frac{N}{U_0} = 0.25, 0.5, 0.75, 1.0$ and resolution $N = 600$ for LBGK (run D) and KBC (run E). .... 88

7.4 Effective viscosity ratio $\nu_{eff,k}/\nu$ for simulations A, B, C and E at different time instances. ................................. 90
7.5 Effective viscosity ratio $\nu_{\text{eff},\Omega}/\nu$ for simulations A, B, C and E at different time instances.

List of Figures

2.1 Illustration of advection step on a two-dimensional lattice with 9 populations ($D2Q9$). After the populations are redistributed through the collision, they are streamed along their respective lattice links to the next node. The "rest particle" stays on its node indefinitely.

3.1 Lattice Boltzmann equations as a map of the kinetic-theory parameter $\lambda = \Delta t/\tau$ into the LB interval $\beta \in [0, 1]$ (2.2). 1: Exact (3.19); 2: HCD extension (3.9); 3-6: Polynomial extensions $\varphi_n$ at various $n$; 3: $\varphi_1 (\lambda_1 = 2)$; 4: $\varphi_2$; 5: $\varphi_3 (\lambda_1 \approx 2.51)$; 6: $\varphi_9 (\lambda_1 \approx 4.70)$. $\beta = 0$ corresponds to populations $g_i$; $\beta = 1/2$ corresponds to the equilibrium populations $g_{i}^{\text{eq}}$; $\beta = 1$ corresponds to the mirror populations $g_{i}^{*} = 2g_{i}^{\text{eq}} - g_{i}$; Over-relaxation range is $1/2 < \beta < 1$; Shadowed strip $\beta \in [0.99, 1]$ indicates typical operation domain of LB simulations. Curves 2, 3, 5 and 6 extend into the over-relaxation sub-interval $\beta \in [1/2, 1]$.

4.1 (a) Turbulent flow generated by a round cylinder. Snapshot of the vorticity iso-surfaces are shown, colored with the effective viscosity. Blue: $R > 0$ (dampers); Red/Yellow: $R < 0$ (promoters). The interplay between the dampers and promoters along each vortex tube is clearly visible. (b) Snapshot of the intertwining of dampers ($R > 0$, blue) and promoters ($R < 0$, red). Essential dampers ($R > 1.5$) and promoters ($R < -0.6$) are shown. The entropic feedback is concentrated in the region behind the obstacle, where the transition to turbulence occurs. Gray background: Vorticity.
4.2 Distribution of the time-averaged normalized effective viscosity \( R = (\nu_{\text{eff}} - \nu) / \nu \) at the mid-section of the flow past a round cylinder. Red/Yellow: Promoters \((R < 0)\); Blue: Dampers \((R > 0)\); Green: Nominal \((R = 0)\). While the snapshot in Figure 4.1 demonstrates a larger variation of the effective viscosity, the time-average picture is much milder: most of the activity (strongest damping neighboring the strongest promotion) is concentrated at and around the twin shear layers, just behind the cylinder. In the rest of the domain, the deviation of the effective viscosity from its nominal value is less than a fraction of a percent.

4.3 Top: History of the entropic stretch \( \alpha \) at a monitoring point; Middle: Histogram of \( \alpha \); Bottom: Close-up of the histogram around the dominant value \( \alpha = 2 \).

5.1 Illustration of the mirror states of KBC, ELBM and the standard LBGK. The dashed lines indicate iso-contours of the constrained convex \( H \)-function with the local equilibrium at its minimum. LBGK uses a fixed relaxation by over-stepping the equilibrium exactly once. The ELBM searches for a mirror state along the same direction, but applies the isentropic condition \( H[f] = H[f_\text{mirr}] \). The KBC method uses an over-relaxation for the \( s \)-part, but searches for the minimum entropy value along the \( h \)-direction.

5.2 Illustration of a lattice node \((x_b)\) in proximity of a solid wall (shaded area). Missing populations (dashed arrows) are provided by the boundary condition.

6.1 Convergence rate for Green-Taylor vortex at \( t = t_c \). LBGK (solid black line), KBC A (blue dashed line), KBC B (green cross symbol), KBC C (magenta dotted line), KBC D (orange square symbol), ELBM (red circle symbol), second order convergence (fine dotted line).

6.2 Decay of Green-Taylor vortex for times \( t = t_c, 2t_c, 3t_c \) and \( N = 128, Re = 100, u_0 = 0.03 \). Symbols for simulations as in Figure 6.1, analytical solution: light solid. Results represented by symbols have been sub-sampled for clarity.

6.3 Roll up of the double shear layer at a grid size of \( N = 512 \) and Reynolds number \( Re = 30000 \) for model KBC-A.
6.4 Vorticity field at $t = t_c$ for $\kappa = 80, u_0 = 0.04$. Columns: LBGK, KBC A, KBC B, KBC C, KBC D, ELBM, respectively, rows: Resolution $N = 128, 256, 512$. ........................................ 65

6.5 Convergence rate for doubly periodic shear layer at $t = t_c$ and $Re = 30000, \kappa = 80, u_0 = 0.04$. Symbols for simulations as in Figure 6.1, second order convergence (fine dotted). Error with respect to reference solution (LBGK at $N = 2048$ resolution). ... 65

6.6 Evolution of kinetic energy and enstrophy (mean: left axis and large symbols, standard deviation: right axis and smaller symbols). Symbols for simulations as in Figure 6.1, results represented by symbols have been subsampled for clarity. ............... 66

6.7 History of the total entropy in the simulation of the double shear layer. Solid: KBC-A; Dashed: ELBM; Dotted: KBC-A with $\gamma = 1$; Dash-dotted: LBGK. Grid size: $L = 128$; Reynolds number $Re = 30000$. ............................................ 66

7.1 Vorticity field for decaying two-dimensional turbulence $Re = 13'134, N = 1024$, for LBGK (first row) and KBC B (second row) and times $t/t_e = \{10, 20, 40, 60, 80, 100\}$ from left to right. ............ 71

7.2 Evolution of kinetic energy and enstrophy for $Re = 13'134$. Mean: left axis and large symbols, standard deviation: right axis and smaller symbols. Symbols for simulations as in Figure 6.1, results represented by symbols have been sub-sampled for clarity. ....... 73

7.3 Evolution of palinstrophy (left column, mean: left y-axis, large symbols, standard deviation: right y-axis, small symbols) and mean stabilizer $\gamma$, mean entropy $S$ (right column, left y-axis, large symbols and right y-axis, small symbols, respectively) for $Re = 13'134$. Symbols for simulations as in Figure 6.1, results represented by symbols have been sub-sampled for clarity. ...... 74

7.4 Energy and enstrophy spectra for two-dimensional turbulence at $Re = 13'134$ for $N = 1024$ at time $t/t_e = 50$. Symbols for simulations as in Figure 6.1, results represented by symbols have been sub-sampled for clarity. .................. 75

7.5 Evolution of kinetic energy, enstrophy, palinstrophy and stabilizer $\gamma$ for $Re = 1.5 \cdot 10^5$ at resolution $N = 4096$. Mean: left y-axis and large symbols, standard deviation: right y-axis and smaller symbols. Symbols for simulations as in Figure 6.1, results represented by symbols have been sub-sampled for clarity. ...... 76
7.6  Energy and enstrophy spectra for two-dimensional turbulence at $Re = 1.5 \cdot 10^5$ for $N = 4096$ at time $t/t_e = 50$. Symbols for simulations as in Figure 6.1, results represented by symbols have been sub-sampled for clarity. ............................................. 77

7.7  Vorticity field for decaying two-dimensional turbulence, $Re = 1.6 \cdot 10^6$ for time $t/t_e = 50$. ................................................................. 78

7.8  Evolution of enstrophy for $Re = 1.6 \cdot 10^6$ at resolution $N = 1024$ (a) and $N = 4096$ (b). Mean: left y-axis and large symbols, standard deviation: right y-axis and smaller symbols. Symbols for simulations as in Figure 6.1, results represented by symbols have been sub-sampled for clarity. In (a) the dark dashed line represents the corresponding values at $N = 4096$ for LBGK. ............ 79

7.9  Energy and enstrophy spectra for two-dimensional turbulence at $Re = 1.6 \cdot 10^6$ for $N = 1024, 2048, 4096$ at times $t/t_e = 50$. Symbols for simulations as in Figure 6.1, results represented by symbols have been sub-sampled for clarity. ............................................. 80

7.10 Iso-surface of vorticity component $\omega_z = 0$ at time $t = 0.5$ colored with velocity magnitude rendered at $z = 0$, $x,y \in [0,\pi]$ plane. Runs A ($N = 100$), B ($N = 200$), C ($N = 400$) and D ($N = 600$, reference solution). ....................................................... 82

7.11 Mean enstrophy and kinetic energy evolution with time for simulations A (⋯), B (−⋯), C (⋯) and D (−). Gradients evaluated with second-order of accuracy. ................................. 84

7.12 Kinetic energy density spectrum and cumulative distribution function of the energy-dissipation rate density $D(\kappa)$ at time $t = 0.5$. Symbols as in Figure 7.11. ......................... 85

7.13 Second order longitudinal structure function and longitudinal and transverse velocity correlation at $t = 0.5$. Symbols as in Figure 7.11. ................................. 85

7.14 Spatial and temporal distribution of the stabilizer $\gamma$. .................. 86

7.15 Mean (symbols) and r.m.s. fluctuations (error bars) of the compressibility $\nabla \cdot u$ for runs D (LBGK, open symbols) and E (KBC-N4, full symbols) with time. Gradients evaluated with second-order of accuracy. ................................. 89

7.16 Turbulence kinetic energy spectrum and longitudinal and transversal velocity correlation function at $Re_\lambda = 564$, $t = 0.075$ (solid) and initial values at $Re_\lambda = 2000$ (dashed). ................................. 91
8.1 Instantaneous vortex structures in the turbulent channel flow at $Re_{\tau} = 180$ (KBC-C2). ........................................... 97
8.2 Average stream-wise velocity and r.m.s. velocity fluctuations in wall units in the simulation of the turbulent channel flow at $Re_{\tau} = 180$. Symbol: KBC-C2; Solid line: DNS data [138]. The log-law of wall (dashed) is shown to guide eye. ........................................... 98
8.3 Average stream-wise velocity and r.m.s. velocity fluctuations in wall units in the simulation of the turbulent channel flow at $Re_{\tau} = 590$. Symbol: KBC-C2; Solid line: DNS data [138] .......... 98
8.4 Instantaneous vortex structures in the turbulent pipe flow. .......... 99
8.5 Mean velocity component in flow direction for the turbulent pipe flow. KBC-N1. .................................................. 100
8.6 Rms velocity profiles for the turbulent pipe flow. See Fig. (8.5) for the legend. .................................................. 101
8.7 Simulation set-up for the flow past a circular cylinder with diameter $D$. .................................................. 102
8.8 Scaling of the mean drag coefficient and Strouhal number with Reynold’s number for the flow around a circular cylinder. KBC-N1 model for $D = 10$ (orange circles), and $D = 20$ (red squares). .. 103
8.9 Comparison of low-order statistics for the flow around a circular cylinder for $Re = 140000$ with KBC-C2. Lines: Simulation; Shaded: Experiment [153]. .................................................. 104
8.10 Dimensions of the reference car and the computational domain. 105
8.11 Mean and r.m.s. velocity at the symmetry plane $y = 0$ for the turbulent flow around the Ahmed body, $-\ KBC, \circ$ Experiment. .. 108
8.12 Mean velocity vectors $(u_y, u_z)/u_\infty$ at the slant and in the wake of the Ahmed body, $-\ KBC, -\ Experiment$. ............................ 109
8.13 Pressure coefficient, vortex structures and velocity profiles for the turbulent flow around a sphere at $Re = 3700$; comparison to Kim and Durbin [182], Rodriguez et al. [183] and Yun, Kim & Choi [184]. Source: Dorschner et al. [134]. ............................ 110
8.14 Instantaneous vortex ring formation and multi-cycle averaged mean and r.m.s. velocity profiles in a engine-like piston valve assembly at 90° crank angle. Source: Dorschner et al. [117]. 111
8.15 Transitional Flow around the SD8003 airfoil at Reynolds number $Re = 6 \cdot 10^4$ and angle of attack $\alpha = 4^\circ$. Source: Dorschner et al. [187]. .................................................. 112
9.1 Conjugate heat transfer in the turbulent flow over a wall-mounted matrix of cubes at $Re = 3854$. Source: Pareschi et al. [190].

9.2 Confirmation of Laplace’s Law with KBC and LBGK for various values of the surface tension parameter $\kappa$, where the surface tension $\sigma$ increases with increasing $\kappa$.

9.3 Comparison of droplet shapes with experimental results [200] (top) and KBC simulation (bottom) for a binary head-on collision of two unequal sized droplets at Weber number $We = 52.8$.

9.4 Top: instantaneous spatial density distribution; Bottom: instantaneous spatial distribution of the stabilizer $\gamma$. Departure from LBGK value $\gamma = 2$ is visible mainly at the liquid-vapour interface.

9.5 Speed of sound in a binary mixture. Measurements were obtained from a 2D shock tube simulation. The circles and continuous line show the measured and theoretical results, respectively. A molar mass ratio of $m_B / m_A = 4$ was used.

9.6 Binary diffusion started with initial condition given in Eq. (9.111). Shown is the molar fraction of component $A$ at time $t = 1000$ for different Schmidt numbers: $Sc = 0.1$ (circles), $Sc = 1$ (squares) and $Sc = 10$ (diamonds). The kinematic viscosity is $\nu = 0.2$, the mass ratio $m_B / m_A = 4$. The continuous lines show the analytical solutions.

9.7 Binary diffusion with $Sc = 1$, $m_B / m_A = 2$ and $\nu = 10^{-3}$. The simulation with entropic stabilization (continuous line) is stable at the initial discontinuity while the unstabilized solver (dashed line) is not.

9.8 Exponential growth of a small single-mode perturbation in the RTI. For the simulation, we chose $A = 0.243$, $m_B / m_A = 2$, $g = 0.0002$, $\nu = 0.05$, $\rho_L = X m_A + (1 - X) m_B$ and $\rho_U = (1 - X) m_A + X m_B$ with $X = 0.865$. The symbols show our results for $Sc = 0.2$ (circles), $Sc = 1$ (squares) and $Sc = 100$ (diamonds). The continuous lines show LST results with the growth coefficient from Eq. (9.115) and fitted constant $\psi$. The dashed line is the inviscid and immiscible LST result.

9.9 Example simulation of the RTI at $A = 0.133$, $m_B / m_A = 2$, $\nu = 0.05$ and $Sc = 10$ at a grid resolution of $1018 \times 4072$. From left to right, the situations at $t = 10000$, $t = 20000$ and $t = 30000$ are given.
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Publications


