1. Introduction

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1.1 Preface

Lattice-gas cellular automata (LGCA)[1] and even more lattice Boltzmann models (LBM) are relatively new and promising methods for the numerical solution of (nonlinear) partial differential equations. Each month several papers appear with new models, investigations of known models or methodically interesting applications. The field of lattice-gas cellular automata started almost out of the blue in 1986 with the by now famous paper of Frisch, Hasslacher and Pomeau. These authors showed, that a kind of billiard game[2] with collisions that conserve mass and momentum, in the macroscopic limit leads to the Navier-Stokes equation when the underlying lattice possesses a sufficient (hexagonal in two dimensions) symmetry. A few years later lattice Boltzmann models arose as an offspring of LGCA. Their higher flexibility compared to LGCA led to artificial microscopic models for several nonlinear partial differential equations including the Navier-Stokes equation.
I have followed the exciting development of both methods since 1989 and from time to time have given courses on this topic at the Department of Physics and Electrical Engineering at the University of Bremen (Germany). The present book is an extended version of my lecture manuscript.
The word 'introduction' in the title implies two things. Firstly, the level of presentation should be appropriate for undergraduate students. Thus methods like the Chapman-Enskog expansion or the maximum entropy principle which are usually not taught in standard courses in physics or mathematics are discussed in some detail. Secondly, in an introduction many things have to be left out. This concerns, for instance, models with several colors which allow the simulation of multiphase flows[3] or magnetohydrodynamics. Only a few applications of LGCA or LBM to physical problems can be considered. Interesting topics like the divergence of transport coefficients in 2D are not discussed. The interested reader will find, however, references pointing to original articles (especially in the 'What else?' sections).
The lattice-gas cellular automata require special programming techniques which are only sparsely discussed in the widely scattered literature. The book will hopefully fill a gap in this respect (see Subsections 3.1.2, 3.1.4, 3.2.2). Several program codes will be made available via internet (http://www.awi-bremerhaven.de/Modelling/LGCA+LBM/index.html).
Many mathematical text books and courses contain lots of definitions, theorems and proofs - and not much else. In this respect the current book is rather 'unplugged': the emphasis is more focused on presenting the main principles

[1] The abbreviations are explained in Table 6.6.5 on page 270.
[2] Goldenfeld and Kadanoff (1999) compare the time development of lattice-gas cellular automata with a square dance.
[3] When I had almost finished my manuscript I became aware of the wonderful book by Rothman and Zaleski (1997). Simulation of multiphase flows is a major topic in that book.

and not on teaching proof techniques. Nonetheless the proofs of several essential theorems are presented in detail.
Last but not least, I would like to add a few comments on the exercises. Problems with one star ($*$) should be very easy to solve (in a few minutes); those with two stars require more thinking or somewhat lengthy ('... after some algebra ...') calculations. Exercises with three stars are very different. Some of them require quite a bit of programming; others address more advanced stuff which has not been treated here. And finally, some of the three star exercises point to open problems which I have not solved myself.

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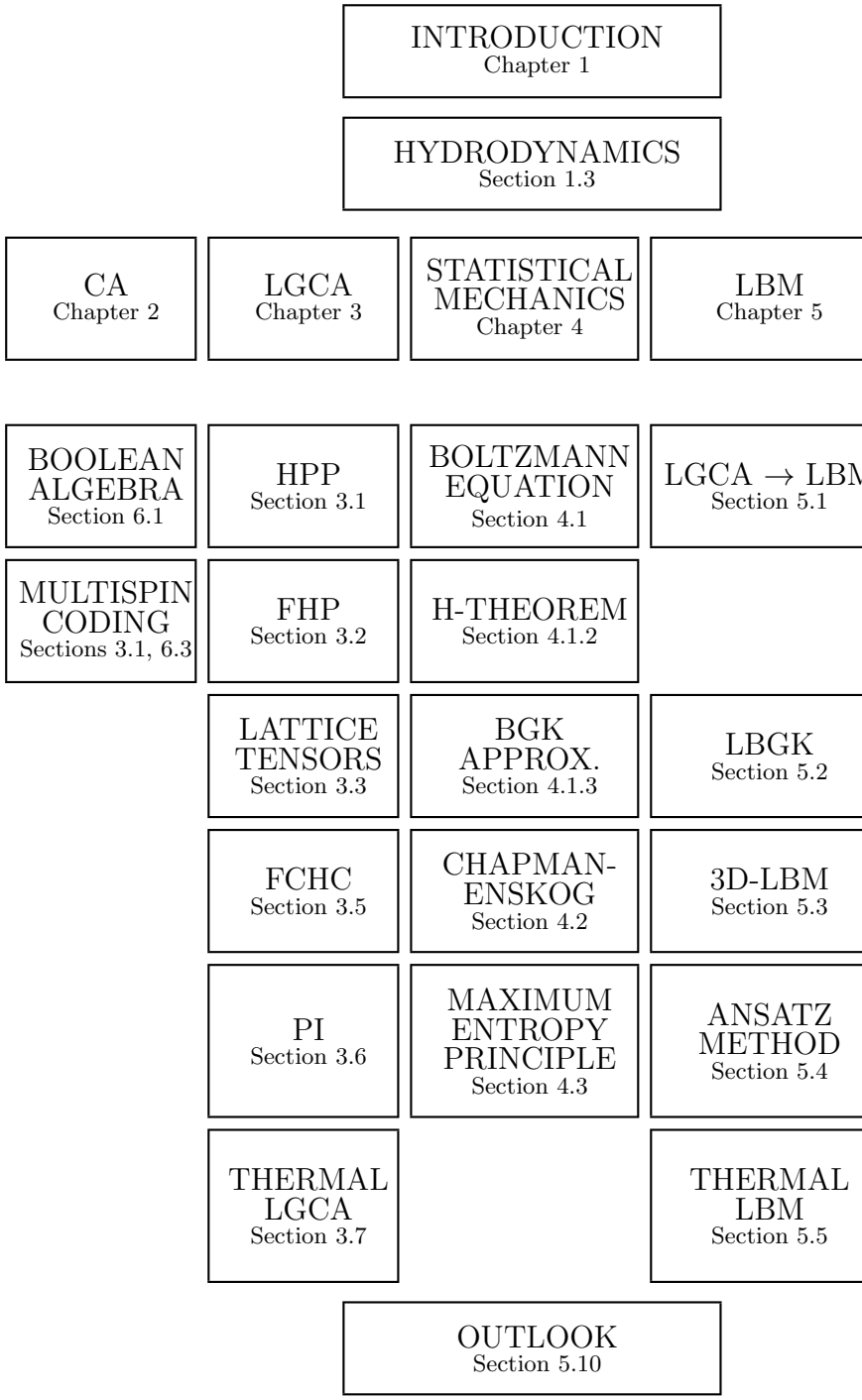
1.2 Overview

The plan of the book is as follows (compage Fig. 1.2.1). In an introductory section the Navier-Stokes equation and several approaches to solve it are discussed. In Chapter 2 cellular automata (CA) are treated in some detail in order to show the special character of lattice-gas cellular automata. CA rules are usually not restricted by conservation laws which is a nice feature when simulating growth processes. The spatial propagation of properties is part of the local updating rule. In contrast, lattice-gas cellular automata obey certain conservation laws and the updating is splitted into a local 'collision' and a propagation to the nearest-neighbor sites. This splitting makes it easier to construct models with desired macroscopic properties. The CA chapter can be skipped in first reading.
Chapter 3 on lattice-gas cellular automata starts with the historically first LGCA, namely the HPP model. This is the simplest model that aimed to simulate the Navier-Stokes equation (but failed to do so!). The emphasis here is on a discussion without digging too much into theory. Special programming techniques like multi-spin coding are explained in detail.
The FHP model is the first successful LGCA. Starting from the Boolean microdynamics the macroscopic equations will be derived up to first order (Euler equation) by a multi-scale expansion (Chapman-Enskog). The second order which yields the Navier-Stokes equation will be addressed later on in the chapters on statistical mechanics (Section 4.2) as well as in the one on lattice Boltzmann models (Section 5.2.3).
The difference between failure (HPP) and success (FHP) depends on the symmetry of the underlying lattice. The tensor of rank four formed from products of the lattice vectors is part of the advection term and has to be isotropic. The main problem in proposing a LGCA for simulations of flows in three dimensions is to find a lattice with sufficient symmetry. In Section 3.3 the lattice tensors of rank two and four for several lattices will be calculated and investigated for isotropy.
If one restricts oneself to single-speed models the only lattice feasible for three-dimensional simulations is the four-dimensional face-centered hypercube (FCHC). Several possible collision rules for this model are outlined in Section 3.5. As an alternative to FCHC multi-speed models are available. When the collision rules are carefully chosen these models conserve energy in addition to mass and momentum and therefore are called thermal models (Section 3.7). Another alternative for simulation in 3D is the pair-interaction (PI) model (Section 3.6). The collision rules of this model are simple in 2D as well as in 3D and thus allow coding using bit-operators.
In Chapter 4 some relevant concepts from statistical mechanics are discussed. Specifically the Boltzmann equation, its five collision invariants, and its (global) equilibrium distribution (Maxwell-Boltzmann) are presented. The chapter contains a proof of Boltzmann's famous H-theorem. For many ap-

plications the complicated collision integral can be substituted by a relaxation toward equilibrium by a term that is proportional to the deviation of the actual distribution from its (local) equilibrium. With this so-called BGK approximation it is possible to derive the Navier-Stokes equation by the Chapman-Enskog expansion on few pages (Section 4.2). In addition, this chapter contains a section on the maximum entropy principle which will be applied later on in the derivation of equilibrium distributions for lattice Boltzmann models.
Chapter 5 is devoted to lattice Boltzmann models. This chapter is almost selfcontained. Readers who are only interested in LBMs (and not in LGCA) can start here but should read at some point Section 3.3 on lattice tensors. However, some remarks in this chapter only make sense to those who are familiar with LGCA.
In Section 5.1 some problems with LGCA are listed and the transition from LGCA to LBM is sketched. The section on the D2Q9 model is in some respect the pendant to the FHP[4] section in Chapter 3 in that this BGK model is discussed in full detail. The equilibrium distributions are calculated from the maximum entropy principle, the Navier-Stokes equation is derived by Chapman-Enskog expansion and implementations of various boundary conditions are discussed. This model is applied to ocean circulation in Section 5.7. The stability of the D2Q9 and other LBMs is discussed in Section 5.6.
Although the use of the maximum entropy principle is a very elegant method, it hides the much wider freedom in choosing equilibrium distributions. Alternatively, one may start from a reasonable ansatz for the distributions and then fix the free parameters during or after the multi-scale expansion such that the desired equations (Navier-Stokes or other partial differential equations) are obtained (Section 5.4).
This ansatz method is used to derive LBMs for diffusion equations (linear as well as nonlinear in any number of dimensions) in Section 5.8. These models can easily be extended to LBMs for reaction-diffusion equations. With the same methods thermal LBMs can be constructed (Section 5.5). LBMs for simulation in 3D are described in Section 5.3. The appendix contains a section on Boolean algebra, some lengthy calculations and code listings of FHP collision rules.

[4] Although the underlying lattices are different!

Fig. 1.2.1. *Overview*



1.3 The basic idea of lattice-gas cellular automata and lattice Boltzmann models

Lattice-gas cellular automata (LGCA) and lattice Boltzmann models (LBMs) are methods for the simulation of fluid flows[5] *which are quite distinctive from molecular dynamics (MD) on the one hand and methods based on the discretization of partial differential equations (finite differences, finite volumes, finite elements, spectral methods) on the other hand. Here the basic idea of LGCA and LBM will be sketched and the differences compared to other methods will be outlined.*

1.3.1 The Navier-Stokes equation

The flow of incompressible fluids can be described by the Navier-Stokes equation[6]

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\boldsymbol{\nabla})\boldsymbol{u} = -\boldsymbol{\nabla} P + \nu \nabla^2 \boldsymbol{u} \tag{1.3.1}$$

together with the continuity equation[7]

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0 \tag{1.3.2}$$

where $\boldsymbol{\nabla}$ is the nabla operator, $\boldsymbol{u}$ is the flow velocity, $P = p/\rho_0$ the kinematic pressure, p the pressure, ρ_0 the constant mass density and ν the kinematic shear viscosity. Different fluids like air, water or olive oil are characterized by their specific values of mass density and viscosity ($\nu_{\text{air}} = 1.5 \cdot 10^{-5}$ m^2 s^{-1}, $\nu_{\text{water}} = 10^{-6}$ m^2 s^{-1}, $\nu_{\text{olive oil}} = 10^{-4}$ m^2 s^{-1}). Incompressible flows of these fluids obey the same form of equation (Navier-Stokes) whereas their microscopic interactions are quite different (compare gases and liquids!). The Navier-Stokes equation is nonlinear in the velocity $\boldsymbol{u}$ which prohibits its analytical solution except for a few cases. Numerical methods are required to

[5] ... and several other processes which can be described on the macroscopic level by partial differential equations ...

[6] The viscous term of the equation was derived in different ways by Claude Louis M. H. Navier (1785-1836) and Sir George Gabriel Stokes (1819-1903). The Navier-Stokes equation in tensor notation reads:

$$\partial_t u_\alpha + u_\beta \partial_{x_\beta} u_\alpha = -\partial_{x_\alpha} P + \nu \partial_{x_\beta} \partial_{x_\beta} u_\alpha .$$

[7] $\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$ is derived from the general continuity equation

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}) = 0$$

by setting $\rho =$ constant.

simulate the time evolution of flows. On the other hand, the nonlinear advection term is most welcome because it is responsible for many interesting phenomena such as solitons (nonlinear waves), von Karman vortex streets (regular vortex shedding behind an obstacle) or turbulence.

The Reynolds number and dynamic similarity of flows. Flows with small velocities are smooth and are called laminar. At very high velocities they become turbulent. The transition from laminar to turbulent flows does not depend only on velocity as will be shown below. Consider the flow past an obstacle, such as a sphere, a cylinder or a plate. What are the characteristic scales of the flow? Obviously the flow field will depend on the (unperturbed) upstream speed U and the linear size (diameter L) of the obstacle. The fluid is characterized by its kinematic viscosity ν. The three parameters U, L and ν have dimensions [length time^{-1}], [length] and [length^2 time^{-1}]. It is easy to see that from these parameters one can form essentially one dimensionless number, namely the Reynolds number

$$R_e = \frac{UL}{\nu}. \tag{1.3.3}$$

The parameters U and L can be used to scale all quantities in the Navier-Stokes equation (the primed quantities are measured in units of U and L): $\boldsymbol{u}' = \boldsymbol{u}/U$, $\boldsymbol{x}' = \boldsymbol{x}/L$, $\boldsymbol{\nabla}' = L \cdot \boldsymbol{\nabla}$, $\nabla'^2 = L^2 \cdot \nabla^2$, $t' = t \cdot U/L$ (the advection time scale L/U is the time for the unperturbed flow to pass the linear size of the obstacle), $P' = P/U^2$ (the kinematic pressure has the dimension of energy per mass). Inserting the scaled quanties into the Navier-Stokes equation leads to

$$\frac{\partial \boldsymbol{u}'}{\partial t'}\frac{U^2}{L} + \left(\boldsymbol{u}'\boldsymbol{\nabla}'\right)\boldsymbol{u}'\frac{U^2}{L} = -\boldsymbol{\nabla}'P'\frac{U^2}{L} + \nu\nabla'^2\boldsymbol{u}'\frac{U}{L^2}$$

or after division by U^2/L

$$\frac{\partial \boldsymbol{u}'}{\partial t'} + \left(\boldsymbol{u}'\boldsymbol{\nabla}'\right)\boldsymbol{u}' = -\boldsymbol{\nabla}'P' + \frac{1}{R_e}\nabla'^2\boldsymbol{u}'. \tag{1.3.4}$$

The scaled Navier-Stokes equation equation (1.3.4) does not contain any scale and only one dimensionless quantity, namely the Reynolds number. Thus for a given type of flow (say the flow past a sphere) the scaled velocity of a stationary flow will depend only on the scaled spatial coordinate and the Reynolds number:

$$\boldsymbol{u}' = \frac{\boldsymbol{u}}{U} = f_u\left(\frac{\boldsymbol{x}}{L}, R_e\right) \tag{1.3.5}$$

where the function f_u depends on the geometry of the problem (the type of flow). The same is true for the scaled pressure:

$$P' = \frac{P}{U^2} = f_P\left(\frac{\boldsymbol{x}}{L}, R_e\right). \tag{1.3.6}$$

Thus all flows of the same type but with different values of U, L and ν are described by one and the same non-dimensional solution ($\boldsymbol{u}'$, P') if their Reynolds numbers are equal. All such flows are said to be *dynamically similar*.
The value of the Reynolds number provides an estimate of the relative importance of the non-viscous and viscous forces. The pressure gradient usually plays a passive role, being set up in the flow as a consequence of motions of a rigid boundary or of the existence of frictional stresses (Batchelor, 1967). Thus the flows can be characterized by the relative magnitudes of advection and viscous forces:

$$\frac{|(\boldsymbol{u}\boldsymbol{\nabla})\,\boldsymbol{u}|}{|\nu\nabla^2\boldsymbol{u}|} \approx \frac{U^2/L}{\nu U/L^2} = \frac{U\cdot L}{\nu} = R_e. \tag{1.3.7}$$

Flows with small Reynolds numbers ($R_e \ll 1$) are laminar, von Karman vortex streets are observed at intermediate values ($R_e \approx 100$) and turbulent flows occur at very high Reynold numbers ($R_e \gg 1$). The fact that flows can be characterized by R_e and the *law of dynamic similarity* were first recognized by Stokes (1851) and Reynolds (1883).
The law of dynamic similarity provides the link between flows in the real world where length is measured in meters and the simulation of these flows with lattice-gas cellular automata and lattice Boltzmann models over a lattice with unit grid length and unit lattice speed. In these models the viscosity is a dimensionless quantity because it is expressed in units of grid length and lattice speed. These dimensionless flows on the lattice are similar to real flows when their Reynolds numbers are equal.

1.3.2 The basic idea

The fact that different microscopic interactions can lead to the same form of macroscopic equations is the starting point for the development of LGCA. In addition to real gases or real liquids one may consider artificial micro-worlds of particles 'living' on lattices with interactions that conserve mass and momentum. The microdynamics of such *artificial micro-worlds* should be very simple in order to run it efficiently on a computer. Consider, for example, a square lattice with four cells at each node such that one cell is associated with each link to the next neighbor node (compare Fig. 3.1.1 on page 41). These cells may be empty or occupied by at most one particle with unit mass $m = 1$. Thus each cell has only two possible states and therefore is called a *cellular automaton*. Velocity and thereby also momentum can be assigned to each particle by the vector connecting the node to its next neighbor node along the link where the particle is located. These vectors are called lattice velocities. The microscopic interaction is strictly local in that it involves only particles at a single node. The particles exchange momentum while conserving the mass and momentum summed up over each node. After this *collision*

each particle propagates along its associated link to its next neighbor node. The microdynamics consists on a repetition of collision and propagation. Macroscopic values of mass and momentum density are calculated by *coarse graining* (calculation of mean values over large spatial regions with hundreds to thousands of nodes).
Do these mean values obey the Navier-Stokes equation? The answer is negative for the model just sketched (discussed in more detail in Section 3.1). This model was proposed by Hardy, de Pazzis and Pomeau in 1973 (HPP model). It took more than 10 years before Frisch, Hasslacher and Pomeau (1986) found the third essential condition in addition to mass and momentum conservation: the lattice has to possess a sufficient *symmetry* in order to ensure *isotropy* of a certain tensor of fourth rank formed from the lattice velocities. In 2D, for example, 4-fold rotational symmetry (square lattice) is not enough whereas hexagonal symmetry (triangular lattice; FHP model; see Section 3.2) is sufficient.
A further condition should be mentioned here. The microdynamics must not possess more invariants than required by the desired macroscopic equations because such so-called *spurious invariants* can alter the macroscopic behavior by unphysical constraints (compare Section 3.8).
The importance of the work of Frisch, Hasslacher and Pomeau (1986) can hardly be overestimated. Their finding of the lattice symmetry condition started an avalanche of LGCA models. Finding a lattice with sufficient symmetry for simulations in 3D was a tough job. Wolfram (1986) showed that lattice tensors over the *face-centered hypercube* (FCHC) are isotropic up to rank 4.

Lattice Boltzmann models were first based on LGCA in that they used the same lattices and applied the same collisions. Instead of particles, LBMs deal with continuous distribution functions which interact locally (only distributions at a single node are involved) and which propagate after 'collision' to the next neighbor node. Coarse graining is not necessary any more. In the beginning this was considered as the main advantage of LBMs compared to LGCA. The next step in the development was the simplification of the collision operator and the choice of different distribution functions. This gives much more flexibility of LBMs, leads to Galilei invariant macroscopic equations without scaling of time, and allows to tune viscosity. Most recently LBMs living on curvilinear coordinate systems have been proposed.

Exercise 1.3.1. (**)
Consider flows that are affected by an external force such as gravity. Discuss the consequences for the similarity of flows. How many independent dimensionless numbers are required to characterize the flow?

1.3.3 Top-down versus bottom-up

The conventional simulation of fluid flows (and other physical processes) generally starts from nonlinear partial differential equations (PDEs). These PDEs are discretized by *finite differences* (Ames, 1977; Morton and Mayers, 1994), *finite volumes* (Bryan, 1969), *finite elements*[8] (Zienkiewicz, and Taylor, 1989 and 1991), or *spectral methods* (Machenhauer, 1979; Bourke, 1988). The resulting algebraic equations or systems of ordinary differential equations are solved by standard numerical methods. Although this 'top-down' approach seems to be straightforward it is not without difficulties. In many textbooks on the numerical solution of partial differential equations the authors put much emphasis on the truncation error which is due to the truncation of Taylor series when going from differential to finite differences whereas physicists are usually more concerned whether or not certain quantities are conserved also by the discretized form of the equations. This latter property is most important for integrations over long time scales in closed domains like, for instance, in the simulation of the world oceans or in coupled atmosphere-ocean models. A small leakage would transform the ocean into an empty basin after some time. *Numerical instabilities* are another problem of this type of numerical methods (Courant, Friedrichs and Lewy, 1928; Phillips, 1956 and 1959).

LGCA and LBM are different variants of the 'bottom-up' approach (Fig. 1.3.1) where the starting point is a discrete microscopic model which by construction conserves the desired quantities (mass and momentum for Navier-Stokes equation). These models are unconditional stable (LGCA) or show good stability properties (LBM). The derivation of the corresponding macroscopic equations requires, however, lengthy calculations (multi-scale analysis). A major problem with the bottom-up approach is to detect and avoid spurious invariants which is, by the way, also a problem for the models derived by the top-down approach. The construction of LGCA or LBM for given macroscopic equations seems to require some intuition. Meanwhile at least for LBM there exists a recipe for the construction of appropriate microdynamics when the conserved quantities of the physical process are known (compare Section 5.4).

1.3.4 LGCA versus molecular dynamics

Another bottom-up approach is *molecular dynamics* (MD) (Verlet, 1967; Evans and Morriss, 1983; Heyes et al., 1985; Mareschal and Kestemont, 1987; Boon and Yip, 1991; Rapaport, 1995). In MD one tries to simulate macroscopic behavior of real fluids by setting up a model which describes the microscopic interactions as good as possible. This leads to realistic equations of

[8] These finite methods can be combined with multigrid techniques; see, for example, Hackbusch (1985).

state whereas LGCA or LBM posses only isothermal relations between mass density and pressure. The complexity of the interactions in MD restricts the number of particles and the time of integration. A method somewhat in between MD and LGCA is *maximally discretized molecular dynamics* proposed by Colvin, Ladd and Alder (1988).

Fig. 1.3.1. *Top-down versus bottom-up (see text).*