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Large Scale Lattice-Boltzmann Simulations: Computational Methods and Applications

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Chapter 1

Computer simulations in fluid dynamics

1.1 Fluid dynamics

A wide variety of applications stemming from the natural sciences and engineering are strongly related with the motion of fluids. Some typical examples are, the atmospheric circulation processes, flow of blood through complex capillary vessels, ground water pollution, compressible flow around an airfoil, and numerous other interesting problems which are of great relevance for the industrial and academic community [1, 2, 3, 4, 5]. A good understanding of the dynamics of fluids is therefore extremely useful in improving several industrial processes and designs, e.g. the wing of an airplane, and may contribute significantly to our knowledge of many fundamental scientific problems, e.g. the impact of hydrodynamics on the morphology of biological growth forms [6].

Although the basic equations for describing the motion of fluids, the so-called Navier-Stokes equations, are known since 1823 [3, 7] a general solution to flow phenomena does still not exist. The extreme complex flow-patterns that may arise are poorly understood. Moreover, a generic approach is hampered by the fact that the equations are often hard to solve [3, 7]. Fluid dynamics is therefore commonly studied by different research areas from their own perspectives and within well-defined restrictions, e.g. incompressible versus compressible flow, creeping versus turbulent flow, single- versus multi-phase flow, Newtonian versus non-Newtonian flow.

A review of the history of fluid dynamics clearly shows that the following approaches are commonly taken in studying these phenomena:

- Experimental measurements.

For many physical systems, it is known that experimental observations elucidate much of their complexities. A well known example in fluid dynamics, is the behavior of fluid flow around a circular cylinder. For increasing Reynolds number * the flow patterns are gradually changing from purely laminar and sym-

*The Reynolds number, Re , is defined as the ratio, $\frac{LV}{\nu}$, where L and V are characteristic length

metric flow to the formation of wakes behind the cylinder and symmetry breaking. After some critical value of the Reynolds number the flow becomes fully turbulent [4, 5, 7]. Similar behavior is observed in flow along a channel. For small Reynolds numbers the velocity profile is known to be parabolic (Poiseuille flow). As the Reynolds number is increased, the velocity profile flattens and the flow becomes fully turbulent beyond some critical Reynolds number [4, 5]. Experiments have indeed contributed significantly to our understanding and knowledge of flow phenomena. Also many relations which are regularly used in engineering applications, for example the drag coefficients for a sphere as a function of the Reynolds number, have been obtained from experimental data [5]. However, the observations are in general only valid for a specific experimental configuration and the experiments may be quite sophisticated and expensive to perform in the case of complex flow applications. Moreover, some phenomena can not be easily observed on the laboratory scale due to the different space and time scales that are present in the dynamics;

- Theoretical methods.

Simplified closure models of the governing equations for a particular flow regime are solved by mathematical methods under the assumption of strict boundary and initial conditions [3]. In principle this approach is preferred because it gives us at least the *hope* to find a somewhat general solution for a class of flow problems. Unfortunately theoreticians have not been able to solve the general behavior of even one of the 'simplest' flow problems, namely flow around a spherical obstacle. In the limit of low Reynolds numbers, the so-called creeping flow regime or Stokes flow, an analytical solution is known to exist, but for moderate to high Reynolds numbers there is no analytical solution known so far [3, 4, 7]. Even low Reynolds number flow in non-trivial geometries is hard to solve by theoretical methods, e.g. fluid flow in a disordered array of cylinders. In general, fluid flow problems are hard to solve analytically due to the nonlinearity of the macroscopic equations and the nature of the (complex) flow boundaries;

- Numerical simulations.

An alternative approach to get insight in flow phenomena is by means of numerical simulations, a research field known as computational fluid dynamics (CFD) [8, 9]. One of the famous examples of this approach is weather forecasting and climate modeling. The objective here is to predict the future state of the atmosphere from knowledge of its present state. In 1922 L.F. Richardson showed that the macroscopic equations for describing the atmospheric circulation processes can be approximated by a set of algebraic difference equations at a finite number of points in space [10, 11]. In CFD this process is known as the discretization of a continuum model. At that time high speed computers were not available and Richardson estimated that a work force of 64.000 people would be required to describe in real time the weather on a global basis. He

and velocity scales and ν is the kinematic viscosity of the fluid. For an incompressible flow in a given geometrical shape of the boundaries, the Reynolds number is the only control parameter.

performed an example forecast by hand using two grid points, but the results were very discouraging. After this failure, numerical prediction was not again attempted for many years. Later, the development of digital computers after the World War II, made the enormous computation power required in a numerical forecast feasible. But due to numerical instability there were still problems with Richardson's equations [11]. Around 1950 J.F. Charney simplified the dynamical equations using several assumptions and derived the so-called quasi-geostrophic model [11]. This model was used to perform the first numerical forecast. Nowadays, with the development of more powerful computers and more sophisticated modeling techniques it is possible to simulate models which are quite similar to Richardson formulation.

The last example clearly illustrates that the success of numerical simulations depends on refinements on the level of the *physical model*, the *numerical schemes* and the available *computational resources*. More specifically stated, in the physical model the different processes are commonly represented by macroscopic equations in which many phenomena are ignored. The numerical schemes have a finite accuracy and are often conditionally stable. And finally the resolution of the grids depends on the available computational resources. Numerical simulations as an intermediate approach for studying fluid dynamics can be useful for problems which are intractable by theoretical methods and are difficult, dangerous and expensive to be observed in real experiments. Also some studies focus on a forecast of a phenomenon and must be performed before the real physical processes actually take place. However, a numerical simulation is only an approximation of a simplified model of the real phenomena and it should be emphasized that the simulation results must be interpreted with extreme care. It is therefore very important to rigorously validate the simulations by a thorough comparison with analytically tractable problems and experimental measurements.

In summary, theoretical and experimental approaches may be extremely valuable as a validation of numerical simulations. Moreover, numerical simulations can be used to some extent, to develop new theory and to replace some experiments which are tedious, expensive or even impossible to mimic at the laboratory scale. It is thus evident that all methods have their own favorable approaches and also their limitations.

In this thesis we focus on numerical simulations of fluid flows. We study an alternative computational approach in fluid dynamics that is based on kinetic theory. In the next section, we first briefly discuss the traditional approach that is still widely used in CFD. Then we introduce the main ideas of the mesoscopic particle based models that we use and finally we motivate the outline of the research described in this thesis.

1.2 Computational fluid dynamics

In this thesis we restrict ourselves to single component/phase, incompressible, isothermal and Newtonian fluid flows. Although this is a major simplification of

the general formulation of hydrodynamics, there are still many realistic applications in this flow regime and the nature of these flows may also be extremely complicated. Traditionally, the macroscopic behavior of fluid flow is modeled by means of the Navier-Stokes equations [1, 2, 3, 4, 5]. The main assumption is that at a macroscopic scale, the behavior of fluid motion is not directly influenced by the detailed molecular interactions, but depends on the average motion of many microscopic particles, the so-called continuum limit assumption. Fluid motion can therefore be described by average physical quantities like velocity, pressure, temperature and density. The flow of an incompressible fluid in a given geometry can be described by the classical Navier-Stokes equations [1, 2, 3, 4, 5]

$$\nabla \cdot \mathbf{v} = 0 \quad (1.1)$$

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v} + \mathbf{f}, \quad (1.2)$$

where ρ is the fluid density, \mathbf{v} is the velocity, p is the pressure, ν is the kinematic viscosity and \mathbf{f} is a body force, e.g. the gravity force. The velocity and the pressure are functions of space and time. Eq. 1.1 expresses the conservation of mass. It states that the in- and outflow of mass in a fluid element are balanced. Eq. 1.2 is the Navier-Stokes equation for incompressible fluids which expresses the conservation of momentum. This equation describes the velocity changes in time, due to convection $(\mathbf{v} \cdot \nabla) \mathbf{v}$, spatial variations in pressure ∇p , and viscous forces $\nu \nabla^2 \mathbf{v}$.

The next step in CFD is to discretize the continuum equations. There are many ways to accomplish this goal, namely by means of finite-difference, finite-volume, finite-element or spectral methods. Each of these strategies have their own philosophy for obtaining a set of discrete algebraic equations (more details can be found in e.g. Ref [8]). Finally, the evolution of the flow field is computed by solving the discrete equations constrained by well-defined initial and boundary conditions via an appropriate numerical algorithm. It is important to notice that the different schemes mentioned above, have a number of aspects in common, namely

- spatial dependence. Most simulations are performed on a grid or mesh. To update a certain nodal point information of neighboring points is required;
- temporal dependence. To evolve the flow variables in time, the results may be needed of the current and previous time step(s) (explicit schemes) and in some methods also information of the future state (implicit schemes);
- convergence. As the resolution of the grid or mesh is refined, it is expected that the discrete approximation should converge to the continuum equations.

From this brief description, it is obvious that the traditional approaches in CFD contain the following steps:

- First, the macroscopic balance equations are derived (physical modeling phase);
- Next, the continuum equations and the flow geometry are discretized and a numerical scheme is chosen to solve the discrete model (numerical approximation phase)
- And finally the actual implementation and execution on a computational platform (sometimes including code parallelization) is performed (mapping phase).

One major objection of the traditional CFD approach is that the physical modeling, the numerical approximation and the mapping phases are often completely separate steps. As a consequence this approach may have some drawbacks regarding for example the flexibility to deal with arbitrary geometries, complex flows and code parallelization. In the next section we introduce the basic concepts of a particle based model as an alternative tool for CFD. In this model the physical modeling and the numerical approximation phases are combined. The intuitive microscopic view of fluid flow, *c.f.* particles are moving and interacting, is still present in this model. As a result it possesses some unique advantages, e.g. flexibility to deal with complex boundary conditions, it can be extended relatively easy to deal with complex flows in some cases and it preserves the spatial and temporal locality and thus is ideal for parallel processing. Some of these nice features will become clear in the remainder of this thesis.

1.3 Lattice Gas hydrodynamics

“We have noticed in nature that the behavior of a fluid depends very little on the nature of the individual particles in that fluid. For example, the flow of sand is very similar to the flow of water or the flow of a pile of ball bearings. We have therefore taken advantage of this fact to invent a type of imaginary particle that is especially simple for us to simulate. This particle is a perfect ball bearing that can move at a single speed in one of six directions. The flow of these particles on a large enough scale is very similar to the flow of natural fluids”,
Richard Feynman (Quoted by Rothman and Zaleski in Ref. [12]).

More than 10 years ago, a complete different strategy of modeling fluid dynamics has been proposed, based on cellular automata principles [13]. The main idea of these so called Lattice Gas Automata (LGA) is that fluid flow can be characterized by the average motion of particles on a regular lattice. A nice introduction about LGA is given by Rothman and Zaleski in their recently published book[12].

“In 1986, Uriel Frisch, Brosl Hasslacher, and Yves Pomeau announced a striking discovery. They showed that the molecular, or atomistic, motion within fluids - an extraordinarily complicated affair involving on the order of 10^{24} real-valued

degrees of freedom- need not be nearly so detailed as real molecular dynamics in order to give rise to realistic fluid dynamics. Instead, a fluid may be constructed from fictitious particles, each with the same mass and moving with the same speed, and differing only in their velocities. Moreover, the velocities themselves are restricted to a finite set."

The main difference between LGA and the traditional numerical approaches is that in LGA the physical evolution rules are discrete while in the latter the discretization is performed on the level of the macroscopic flow equations. In both cases however, the same physical conservation laws are valid.

Lattice Gases can be viewed as mesoscopic models which occupy a position between the full molecular dynamics and macroscopic descriptions by means of partial differential equations. Basically, particles move synchronously along the bonds of a lattice (propagation step) and interact locally, constraint to conservation of mass and momentum (collision phase). This update mechanism is illustrated in Figure 1.1.

The first LGA was the so-called HPP model on a square lattice [14, 15]. The main problem with this model is that the hydrodynamic behavior is not isotropic and the method satisfies some unphysical conservation laws, the so-called spurious invariants. Later, it was realized that the connectivity of the lattice is the main reason for these unphysical effects and in a next development, the so-called FHP model (see Figure 1.1) based on a hexagonal lattice, these problems were eliminated.

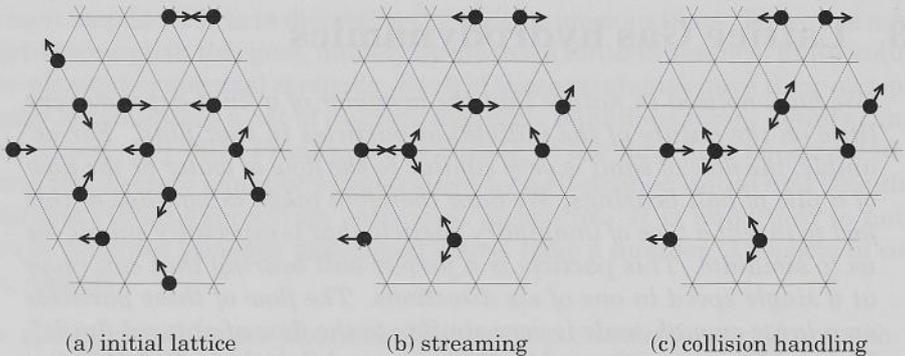


Figure 1.1: Update mechanism of a FHP LGA. Arrows denote a particle and its moving direction. In Figures a to c the propagation (streaming) and collision phases are shown for some initial configuration.

The FHP model evolves according to the following dynamical rule,

$$n_i(\mathbf{x} + \mathbf{c}_i, t + 1) = n_i(\mathbf{x}, t) + \omega_i(\mathbf{n}(\mathbf{x}, t)) \quad i = 1 \dots 6 \quad (1.3)$$

where $n_i(\mathbf{x}, t)$ is a boolean variable representing the presence/absence of a particle with velocity \mathbf{c}_i (unity in the FHP model) at site \mathbf{x} at time t and $\omega_i(\mathbf{n}(\mathbf{x}, t))$

is the output state of the collision operator along link i (the input state is denoted by $\mathbf{n}(\mathbf{x}, t)$). An example of the collision operator that is used in Figure 1.1 is shown in figure 1.2. Notice that in the collision operator only those configu-

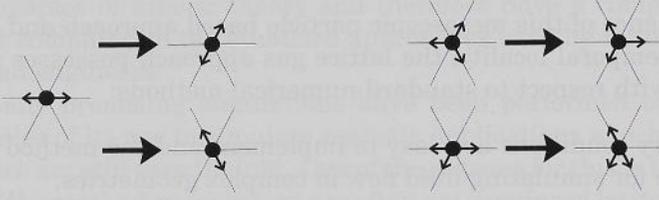


Figure 1.2: Collision rules of the FHP LGA. Arrows denote a particle and its moving direction. When multiple post collision states are possible a random selection is made. The collision rules satisfy mass and momentum conservation.

rations are allowed that satisfy conservation of mass and momentum. For instance, when two particles enter the same site with opposite velocities, both of them are deflected by 60 degrees such that the net momentum in the post collision state remains zero and when multiple post collision states are possible a random selection is made. It can be demonstrated that these microscopic rules simulate the following macroscopic equations [12, 16],

$$\frac{\partial \mathbf{v}}{\partial t} = -(g(\rho) \mathbf{v} \cdot \nabla) \mathbf{v} - \frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v} \quad (1.4)$$

where ρ is the average number of particles per cell and $g(\rho)$ is a function of ρ . For the FHP model $g(\rho) = \frac{\rho-3}{\rho-6}$ [16]. Eq. 1.4 is clearly similar to the Navier-Stokes equations for incompressible fluids, except for the fact that there is a $g(\rho)$ function in front of the convection term. This artifact is known as non-Galilean invariance[†] of LGA. Also in LGA, the density and the velocity are coupled. More specifically stated, flow domains with constant pressure p and a relatively high velocity \mathbf{v} have a higher density ρ than regions with a lower velocity. This is not consistent with the physical behavior of incompressible fluids in which generally very small density fluctuations are present. However, for low velocities or low Mach numbers[‡] $g(\rho)$ can be assumed constant and in Eq. 1.4 the time t , the viscosity ν , and the pressure p can be renormalized ($t' = g(\rho)t$, $\mathbf{v}' = \frac{\mathbf{v}}{g(\rho)}$, $p' = \frac{p}{g(\rho)}$) and the Navier-Stokes equation for incompressible fluids can be recovered.

In summary, a lattice gas automaton is a mesoscopic method for simulation of fluid flow at a macroscopic scale, based on the following observations:

- the macro-dynamics of a fluid is a result of the collective behavior of many particles in the system and details of the microscopic interactions are not essential;

[†]A system is Galilean invariant if the equations do not change when it is observed from a frame of reference that is moving with a constant velocity

[‡]The Mach number, is defined as the ratio, $\frac{V}{C_s}$, with V the characteristic velocity and C_s the speed of sound.

- changes in molecular interactions affect transport properties such as viscosity, but they do not alter the basic form of the macroscopic equations as long as the basic conservation laws and necessary symmetries are satisfied.

As a consequence of this mesoscopic particle based approach and the inherent spatial and temporal locality, the lattice gas approach possesses some unique advantages with respect to standard numerical methods:

- boundary conditions are easy to implement and the method is especially suitable for simulating fluid flow in complex geometries;
- the model is ideal for massively parallel computing because the updating of a node involves only its nearest neighbors;
- the code is extremely simple compared to that of state-of-the-art numerical methods;
- hydrodynamics is modeled in a very intuitive way and in some flow regimes, the method can be easily extended to simulate complex fluids, e.g. multi-component fluids.

1.4 Research motivation and outline

In the previous sections, we described the relevance of hydrodynamics and the different approaches that are regularly used in this field to solve the related problems. The computational fluid dynamics approach is discussed in some more detail. We discussed the basic idea of the traditional numerical modeling strategies in CFD and also introduced the main philosophy of the particle based LGA as an alternative approach in CFD.

The general interest of our research group is in making phenomena from nature tractable for simulation using state-of-the-art parallel processing technology.

In this thesis we consider the potentials for particle based models in CFD. We study the successor of the LGA, the so-called Lattice-Boltzmann models (see chapter 2). Special interest for particle based models is mainly due to the intrinsic locality of their update rules which makes them suitable for efficient simulation on high performance computers. Moreover, a mesoscopic approach to model the macroscopic physics is attractive, because the physics is modeled in an intuitive and natural way.

We approach our research from three different perspectives. Before motivating why in our opinion this approach might be fruitful we first present the different perspectives:

- *Numerical modeling*

Experts in numerical simulations are often interested in new models to effectively study for instance physical systems. The LGA and its successor, the Lattice-Boltzmann method, are relatively new methods for studying fluid dynamics by means of computer simulations. However, these models are based on basic principles of kinetic theory and therefore have a complete different development compared to the standard approaches used by numerical mathematicians and engineers.

Although many promising simulations have been performed based on LGA ideas, examples of its use to simulate realistic applications which are of industrial relevance are still very limited. One of the reasons for this is that due to the simplicity of the method, researchers are often not convinced by its effectiveness in studying complex flow problems. Moreover, as illustrated in the previous sections, LGA models are different from traditional numerical approaches because the physical model and its numerical approximation (including the discretization process) are combined in one cycle. Its understanding and application thus requires knowledge of kinetic theory and fluid dynamics. Finally, LBM simulations have been often used to simulate complex flow behavior at a qualitative level and not many detailed, and thus convincing, validations with experiments and traditional CFD simulations have been published.

In this thesis, we report on rigorous and original studies of lattice-Boltzmann simulations concerning flow in complex geometries and we compare our results in detail with experimental data and other numerical models (see chapter 6). The objective is to get insight in the performance of these particle based models for simulating flow in complex geometries from both a computational point of view and by taking into account the accuracy of the simulation results.

Moreover, we address various important computational aspects that have appeared to be serious shortcomings of LBM. More specifically stated, in chapter 3 we present comparative studies of several boundary conditions and regularly used 3D models. A new technique, to reduce the number of time-steps that are required in lattice-Boltzmann simulations to reach a steady state, is discussed in chapter 4. Extensions of the standard lattice-Boltzmann algorithm from uniform to nested grids are presented in addendum A;

- *Computer Science*

From a computer science perspective we are interested in novel models for large scale complex simulations, that are ideal for execution on the current state-of-the-art high performance machines. We look for models that have intrinsic locality in their update mechanisms. A promising idea in this respect is indeed the philosophy of LGA, that is to allow only nearest neighbor interaction in space and to use explicit time update schemes. Although LGA and LBM models have been claimed to be easy for parallelization, efficient and generic load balancing has not been reported to the best of our knowledge. One obvious reason for this is that in most implementations of LGA and LBM algorithms, the parallelization effort is kept as simple as possible. In chapter 5 we discuss efficient and generic parallelization of lattice-Boltzmann simulations;

- *Physics*

Besides a thorough validation of the lattice-Boltzmann simulation results, we are, from a physics point of view, interested in the hydrodynamic properties of fibrous media. We first study the behavior of the hydraulic permeability as a function of the fiber volume fraction for many ordered and disordered models of fibrous media for a large range of fiber volume fractions and compare our results rigorously with existing theoretical, numerical and experimental data. Furthermore, the functional behavior of the hydraulic permeability is explored in more detail and correlated with the geometry of the media using simple scaling arguments. Finally, we study the effect of wall boundaries on the hydraulic permeability by simulating fluid flow in fibrous media placed between two parallel plates (the so-called bounded media). Although many realistic fibrous media are bounded there are not many theoretical studies reported on this topic. This is mainly due to singularities introduced by the parallel plates. We consider ordered and disordered media and calculate the hydraulic permeability as a function of the distance between the parallel plates and the fiber volume fraction (see chapter 7).

It is obvious that these different perspectives that are used in this thesis require a combined knowledge of hydrodynamics, numerical modeling and computer science. As it became clear from our example focusing on weather forecasting as an application of CFD, the success of computer simulations of large scale complex problems depends on refinements on these three areas. This combined view is indeed the unique and main objective of *computational science* and we believe that especially due to such a typical 'computational scientists' approach, the potentials of new models similar to ideas of LGA can be further explored and developed.