Large Scale Lattice-Boltzmann Simulations: Computational Methods and Applications

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Chapter 8

General discussion

In this thesis we studied several aspects of the lattice-Boltzmann method. In fact we demonstrated that the lattice-Boltzmann method is indeed a versatile tool for the numerical simulation of fluid flow in complex geometries. Briefly stated, several new ideas have been proposed useful for efficient and accurate lattice-Boltzmann simulations. These include an analysis of the commonly used boundary conditions and 3D models, parallelization of lattice-Boltzmann simulations, formulation of a new technique to reduce the number of time steps to reach the stationary state and generalization of the lattice-Boltzmann method on nested grids. Moreover, for a nontrivial benchmark case the lattice-Boltzmann method has been compared thoroughly with the state-of-the-art finite-element method. Finally, the transport properties of various models of (dis)ordered (un)bounded fibrous porous media have been studied in detail. We compared the lattice-Boltzmann results with existing theoretical, numerical and experimental data and made a direct connection between the macroscopic fluid flow and the geometry of the media. The main conclusions are stated separately at the end of each chapter and can also be found in the summary of the thesis.
In this chapter we briefly discuss some interesting and hopefully feasible research topics to be studied in the near future. In Fig. 2.2 of chapter 2 we have summarized the recent developments of the lattice-Gas automata and the lattice-Boltzmann method. In fact there are three main directions in the research of this field. The first one is related to computational aspects, e.g. the extension of lattice-Boltzmann models to non-uniform grids. The second one is about novel lattice-Boltzmann simulations and formulation of new models capable of simulating complex hydrodynamics. And finally, studies on fundamental issues like the theory of lattice-Boltzmann models are still in progress. The following suggestions are quite natural steps to proceed with:

- Application of different formulations of LBM on non-uniform grids to realistic three-dimensional problems. In recent years, several studies have been reported for extending the lattice-Boltzmann method to non-uniform lattices. All these efforts including that of our own are thus far only applied to rather simple geometries. The challenge now is to apply these techniques to realistic cases. Important issues like grid or mesh generation and efficient parallelization will be major difficulties.

- Boundary conditions. Much debate is still going on about boundary conditions for LBM. In fact the major problem of the boundary conditions is that the number of unknown particle densities is higher then the number of constraints (the prescribed density or momentum). Several models have been proposed in the past to deal with this problem consistently. As we have shown in chapter 3 more sophisticated methods may be required in some cases.

- Fast lattice-Boltzmann schemes. One major problem of the LBM is the relatively large number of time steps sometimes required to reach the stationary state. In chapter 4 we proposed an alternative method for reaching a faster convergence. However, this technique is limited to body-force driven flows. Methods based on the numerical solution of the Boltzmann transport equation, as recently been studied by Verberg and Ladd [119], are very promising and must be stimulated.

- Moving boundaries. There are many applications related to fluid flow in dynamically changing geometries. Typical example are suspension flow and blood flow in arteries. Extension of lattice-Boltzmann models to these cases may open a very wide range of potential applications.

- Fluid flow in porous media. The most successful application of the lattice-Boltzmann method is fluid flow in porous media. However, most of the studies are dealing with systems far from the percolation threshold. This is mainly due to computational limitations. The study of fluid flow near the percolation threshold is of fundamental physical interest. For two-dimensional systems these problems might still be feasible using current state-of-the-art parallel computing technology.

- Complex hydrodynamics. Different models have been proposed in the past for simulation of complex hydrodynamics, e.g. multi-phase , thermal and viscoelastic models. In this thesis we studied fluid flow in the SMRX static mixer reactor. We restricted to single-phase, isothermal and Newtonian fluid mechanics. However, in real engineering processes these restrictions may not be appreciated. It is interesting to apply the existing lattice-Boltzmann models for complex hydrodynamics to simulate complex flow in for instance the SMRX reactor. As all existing lattice-Boltzmann models have their limitations, the only way to really see whether these efforts will be successful is by doing it.

- Theory of lattice-Boltzmann models. As we have already noticed in chapter 2 it has been argued by several authors that the lattice-Boltzmann equation is a specific discretization of the Boltzmann transport equations. Existing knowledge of kinetic theory may therefore be very useful in extending the lattice-Boltzmann method to models for simulating complex hydrodynamics and for other methodological improvements.