Modelling of electrokinetic flow using the lattice-Boltzmann method

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Abstract

TODO: Update abstract!

The lattice-Boltzmann method is used to model flow in electrokinetic systems. A modelling approach based on the coupling of Navier-Stokes, Nernst-Planck and Poisson's equation of electrostatics is utilised. Three lattice-Boltzmann methods are formulated for the three equations respectively.

The method is implemented in `C++` with the aim of being high performing. Topics as locality, instruction pipelines and parallel computing are considered. The implementation is tested for a number of classic examples with known solutions, e.g. Taylor-Green vortex flow, an Helmholtz equation and an advection-diffusion situation. The computed solutions agree well with the analytic solutions.

The physical systems modelled consists mainly of various charged channel flows of ionic solutions. Electrokinetic effects, such as electroosmosis and the electrovicous effect are studied. This is done in thin channels where the thickness of the electrical double layers is comparable to the channel dimension. The electroviscous effect is shown to slow the flow down and a local minimum is found in the velocity profile for thick enough double layers. Other more complicated systems are also studied; electroosmotic flow in a channel with heterogeneously charged walls and flow in a an array of charged squares.

Keywords: lattice-Boltzmann, electrokinetics, electrohydrodynamics, Nernst-Planck, Poisson-Boltzmann, high performance computing.

1 Introduction

This thesis deals with modelling of physical problems in the interdisciplinary field of hydrodynamics and electrostatics. The tool used for realising this is the new and promising but somewhat immature lattice-Boltzmann method. This is a method that is still under development but is today used in practical applications both in industry and academy.

1.1 Background

There is currently an ongoing project at the mathematics faculty of Chalmers University in producing a modelling package that should be able to deal with transport of various liquids and particles through complicated structures. The method of choice has fallen upon the lattice-Boltzmann method for its suitable characteristics in the systems of interest.

This work aims to investigate the possibility and procedure for taking electrical effects into account in the modelling of charged fluids. More theoretical questions about the method itself and of the physics involved is of interest as well as how the method may be effectively implemented on a computer.

From both industry and academy, there is a demand on the modelling of this kind of physics. For instance, in medical sciences, accurate modelling of transport of charged fluids is a fundamental ingredient in understanding biological systems and to be able to manipulate them. As a consequence of the always so present desire of more environmental friendly ways of using the planet, automotive industry are now engineering electrical cars. A great challenge is to produce high performing and durable batteries, the ability to accurate model the electrolytes in the batteries is indeed an advantage in achieving this.

1.2 Outline

The text is structured in five main chapters. In chapter **??**, the physics involved and the equations of interest are presented. This is followed by chapter **??** where the lattice-Boltzmann method is formulated for the different equations of interest. Also an introduction to the method as well as some discussion on different boundary conditions is given here. In chapter **??**, the implementation of the method is discussed together with some general aspects that is important to have in mind in order to produce a high performing code. The implementation is then tested for classic examples with known solutions in chapter **??**. Finally some results in electrokintetics are presented and discussed in chapter **??**. Here, the focus is rather on the physics of the simulated systems then on LBM aspects of the problems. These aspects, such as grid dimensions, how LBM parameters relate to physical quanities etc. are discussed for the problems in chapter **??**.

1.3 Previous work

An extensive treatment of both theory and experiments in the field of electrokinetics is carried out in [1]. Mainly the Poisson-Boltzmann model is used in the modelling but

also in some situations, the model used in this work based on the coupling of Navier-Stokes, Nernst-Planck and Poisson's equation of electrostatics is discussed. Also in [2], this modelling approach is used. However, the computational model is not the Lattice-Boltzmann method (LBM).

There are a lot of formulations of the LBM for the Navier-Stokes equations as the method typically is used in the modelling of fluid dynamics. Not so common are formulations for the Nernst-Planck and Poisson's equation. However there are a few, e.g. in [3] and [4] formulations for the Poisson's equation is discussed. In [5] a complete formulation for the three equations are presented together with some example simulations of electrokinetic systems. The formulation presented in [5] will not be completely the same as the one used in this work as is discussed in later chapters of this text.

References

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