Large Scale Lattice-Boltzmann Simulations: Computational Methods and Applications

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Summary

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. 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. Although the basic equations for describing the motion of fluids are known for a long time a general solution to flow phenomena does still not exist.

The Lattice Boltzmann method (LBM) is a relatively new approach for the numerical simulation of fluid flow. In this method fluid is modeled by particles moving on a regular lattice. At each time step the particles propagate to neighboring lattice points and re-distribute their velocities in a local collision phase. This inherent spatial and temporal locality of the update rules makes it ideal for parallel processing. The main objective of this thesis is to study realistic fluid dynamical problems by means of the lattice Boltzmann method on parallel systems. The thesis focusses on computational aspects and new physical insights related to fluid flow in porous media.

In chapter 3 the accuracy of the bounce-back scheme for stair-cased geometries is studied by simulating fluid flow in an inclined tube. Similar to the case of flat walls, a first-order dependence of the relative error on the grid spacing has been found due to the shift of the boundaries. For a specific inclination angle of 45 degrees, the relative error is second-order convergent in lattice spacing when the location of the wall is assumed to lie half-way between the solid nodes and the last fluid nodes. Besides the study related to the bounce-back boundary condition, boundaries for driving a flow between the inlet and outlet of the system are considered. In this context a comparison is made between the well-known body-force approach and pressure boundaries. For low Reynolds numbers and simple geometries a good agreement between these approaches has been found. Apart from the evaluation of the boundary conditions, two common implementations of the lattice-Boltzmann model for $3D$ simulations are studied, the D_3Q_{15} and the D_3Q_{19} models. It is shown that within the D_3Q_{15} model, an unphysical checkerboard effect can be found, which generates spurious conservation of mo-

mentum and mass within two distinct populations of particles. For some stationary flows, this checkerboarding effect generates unphysical patterns in the hydrodynamic fields. However, in the test cases the overall effect of these artifacts is negligible.

Next, parallelization of LBM simulations is revisited. The need for studying this issue, is that often implementation of LBM simulations on parallel systems, is based on decomposition of the computational grid in equal sub volumes (slice and box decomposition). However, it is known that the computational cost of LBM simulations scales linearly with the number of fluid nodes. The obstacle points do not contribute significantly to the total computation time. It is thus obvious that efficient parallelization for a wide range of applications can only be obtained by using appropriate load balancing methods. In this context load balancing of LBM simulations by means of the Orthogonal Recursive Bisection method is studied. For fluid flow in a centrifugal elutriation chamber, a 12 to 60% increase in speed has been gained compared to the slice and box decompositions.

Furthermore, a detailed validation of LBM and traditional finite element methods (FEM) for fluid flow in complex geometries is performed. As a realistic test case fluid flow in a static mixer reactor has been considered. In this validation study the numerical results for the velocity and the pressure of LBM are compared rigorously with FEM calculations and experimental data. A good agreement between both methods and experimental data has been found. It appears that the LBM is less memory consuming and uses computational times comparable to the FEM for the same level of accuracy of the simulations. However, there may be cases where the FEM method is more efficient, e.g. due to the uniform nature of the LBM grids. LBM yields similar accuracy between pressure and velocity fields, whereas the FEM could exhibit a rather good estimate of the velocity field combined with a bad estimate of the pressure field due to mesh coarseness. LBM can therefore be considered as a simple alternative for simulating laminar flow in complex geometries. However, the execution times of the LBM methods show a sharp increase on very fine meshes.

To cope with this shortcoming two refinements on the LBM method are proposed, namely an iterative momentum relaxation (IMR) technique to decrease the number of time steps that are required to reach a steady-state and LBM simulations on nested grids. The IMR technique is based on an iterative adjustment of the local body-force. It has been validated on three test cases, namely fluid flow around a spherical obstacle, flow in random fiber mats and flow in a static mixer reactor. In the first test case the IMR method appears to be around 35 times faster, whereas for the more complicated benchmarks, the IMR method is approximately 3 times faster. Notice that for realistic runs the benefit gained by IMR is still significant. In the second refinement the LBM method has been extended to computational grids consisting of multiple nested grids with increasing spatial resolution. Basically, the discrete velocity Boltzmann equation is solved numerically on each sub-lattice and interpolation between the interfaces is carried out in order to couple the sub-grids consistently. This approach has been validated on the simple Taylor vortex flow benchmark. Although this

work is still quite preliminary the first results are promising. In the near future our aim is to apply this technique to more complicated problems.
In the last chapter, a study on the hydrodynamic properties of fibrous media is presented. Despite the numerous experimental and theoretical studies, the hydrodynamic properties of disordered fibrous porous media are still poorly understood. The existing numerical studies are only valid for dilute systems or they completely neglect the typical disorder of real 3D fibrous media. 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 has been calculated and compared rigorously with existing theoretical, numerical and experimental data. For the ordered media, namely SC and BCC configurations, a good agreement is found between our simulations and existing theoretical and numerical data for the complete range of fiber volume fractions. For disordered fibrous media a good agreement between LBM, the analytical results of Jackson and James and the empirical Kozeny-Carman equation is found in the dilute limit, as expected. Moreover, the results suggest an exponential dependence of permeability on fiber volume fraction in a wide range and this functionality seems to be a generic feature of fibrous porous materials, independent of whether they are random or not.
Using simple scaling arguments, it is argued that there is a strong correlation between the hydraulic permeability and the distance between the fibers. This correlation is further explored and used as a possible explanation of the behavior of the hydraulic permeability as a function of the fiber volume fraction.
Finally, the effect of wall boundaries on the hydraulic permeability has been studied 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. For various wall separation distances the hydraulic permeability is computed for a bi-periodic array of cylinders and a disordered medium as a function of the fiber volume fraction. These results are compared with the effective medium theory of Tsay and Weinbaum. For bounded ordered media a reasonably good agreement is found in the dilute limit. For higher fiber volume fraction the effective medium theory of Tsay and Weinbaum overpredicts the permeability. From the strong correlation between the average fiber-fiber distance and the hydraulic permeability, a phenomenological expression is derived based on the effective medium theory of Tsay and Weinbaum. This correlation appears to be valid for a larger range of fiber volume fractions and can be used for a rapid prediction of the hydraulic permeability of bounded fibrous media.