Multiscale Transport in Microfluidic and Nanofluidic Systems

Introduction

An order-parameter formulation [1] that allows for treatment of multiphase flow and transport, and inclusion of short-range and long-range interactions at solid surfaces is adopted. The lattice Boltzmann method (LBM) provides for an efficient approach to implementing the order-parameter formulation for multiphase flows. Conditions at solid boundaries are relatively easily implemented using the lattice Boltzmann technique, making it well suited for handling complex geometries, and the local nature makes it highly amenable to massively parallel processing. A multiprocessor version for multiphase flows in irregular geometries and three-dimensions has been developed using domain decomposition and MPI (Message Passing Interface) and is being extended for the hybrid approach.

A hybrid continuum-molecular dynamics approach offers several advantages for the study of transport and reactions in microfluidic and nanofluidic systems. The colloid or biomolecule is treated microscopically, and the solvent is taken to obey coarse-grained dynamics. This allows for an efficient treatment of the large differences in time scales between the solvent particles and the colloid particles or biomolecules. The understanding of these hydrodynamic interactions is important in the development of biomimetic sensor devices. Both lattice Boltzmann and finite-volume discretizations of the Navier-Stokes equations will be used for modeling the solvent.

Thread Stability in Microfluidic Geometries

The control of fluid interfaces is often a significant element in microfluidic devices. The order-parameter formulation, solved using a lattice Boltzmann approach, is used to study the stability of a thread of fluid flow focusing device [2], as a function of the capillary number (Ca), the fluid flowrate ratio $\xi=Q_i/Q_o$ and the fluid viscosity ratio $\lambda=\mu_i/\mu_o$.

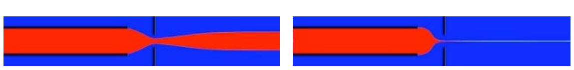

Figure 1. Ca=1×10^{-2}, ξ=0.25: (a) λ=0.5, (b) λ=0.25.

We are currently studying the influence of these parameters on thread stability and drop formation.

Transport of Immiscible Droplets in Converging-Diverging Flow

The ability of the present approach to model droplet deformation in complex geometries is shown by the results of a simulation in a pressure-driven flow in a converging diverging geometry.

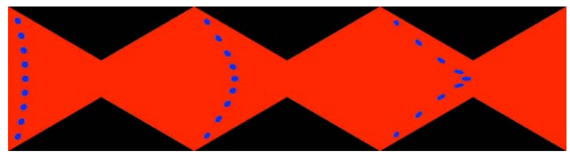

Figure 2. Applied Pressure Gradient (Ca=0.1, λ=1).

Simulation of Electrokinetic Flows

Electrokinetic flows in microfluidic systems are often characterized by Debye lengths much smaller than the characteristic dimensions of the channel. This necessitates use of a composite grid structure, with a fine grid near the solid walls and a coarse grid elsewhere. Our tests of multiblock grids for lattice Boltzmann methods indicate that an alternative approach using finite-volume discretizations on structured overlapping grids offers a more efficient alternative. We have used Overture, an object-oriented framework, for solving partial differential equations with support for finite-difference and finite-volume discretization, composite structured overlapping grids with adaptive mesh refinement, and moving meshes, developed at the Lawrence Livermore National Laboratory, for the solution of the coupled Poisson-Boltzmann equations and Navier-Stokes equation. The use of structured grids allows for an efficient solution using multigrid methods. A parallelized version is available, making the application to complex three-dimensional geometries feasible.

Extensional Flows in Microfluidic Systems

There is considerable interest in generating extensional flows in microfluidic systems [3]. The semi-hyperbolic geometry [4]:

$R^2(z+B)=C$, $C=LR_0 2R_e^2/(R_0^2-R_e^2)$, $B=LR_e^2/(R_0^2-R_e^2)$

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where R_0 and R_e are the entrance and exit dimensions of a die of length L, provides an effective geometry for strongly extensional flows, that has potential for use in microfluidic geomteries. A section of the composite grid used for the semi-hyperbolic channel geometry, with a finer mesh only in the region near solid boundaries to model the EDL, is shown in Figure 3.

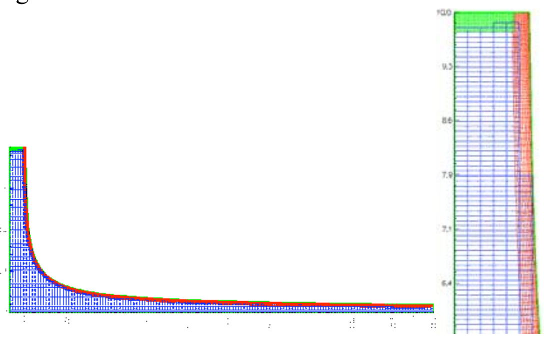

Figure 3. Composite overlapping Grid

The flow parameter $\chi=|E|-|\Omega|/| E|-|\Omega|$ shows a strongly extensional flow character over most of the flow domain.

Dielectrophoretic Particle Transport

Dielectrophoresis provides a powerful method for particle or cell separation in microscale systems. We have modeled the dielectrophoretic transport of tracer particles by solving the coupled Poisson-Boltzmann and Navier-Stokes equations in a separation system [5] in which 5.7μm and 15.7 μm diameter polystyrene microparticles are separated under a potential gradient in a channel with a constriction to produce an inhomogeneous electrical field. Our results are in agreement with the experimental and computational results reported in [5]. However, we would like to avoid the use of semi-empirical correction factors for particle size by the use of a hybrid approach, in which the solvent is modeled using the LBM, with a molecular dynamics (MD) model for the microparticle.

Figure 4. (a) 5.7μm particles (b) 15.7μm particles

Hydrodynamic interactions between the beads and the solvent are implemented through a frictional force proportional to relative velocity between the beads and the surrounding fluid [6]. Due to the dissipative nature of the coupling, stochastic forces with zero mean are added to both the fluid and the beads. This approach offers a significant computational advantage over a purely MD approach.

Conclusions

The LBM provides a computationally efficient technique for the simulation of multiphase flows. A composite overlapping structured grid model using finite-volume discretization provides an efficient technique for the simulation of electrokinetic flows in complex geometries, with a wide separation between the Debye length scale and channel dimensions. A hybrid LBM is under development that will allow for an accurate modeling of hydrodynamic interactions in biomolecular transport in confined geometries.

References

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