Recent Advances of Lattice Boltzmann Method in Microfluidic numerical Simulation

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Abstract. The technology of microfluidics is widely adopted in various fields such as biomedicine, microanalysis, and microelectronics. For example, pharmaceutical scientists often use microfluidics as a tool for drug delivery or cell separation. The LBM (Lattice Boltzmann method) is a commonly used numerical simulation in microfluidic researches. LBM is used extensively for simulations containing complicated boundary conditions and multiphase interfaces as it needs relatively low computing power compared to other numerical simulation methods in complex situations. The brilliant capability in parallelism also allows it to have a high multitasking performance, increasing overall efficiency. In this paper, we reviewed several typical applications of LBM in the following three fields: (1) particle regulation; (2) flow control; (3) drug delivery. We concluded defects in current studies and proposed potential improvements to be investigated in the future.

1. Introduction
Microfluidics is widely used in cell separation [1] and drug delivery [2]. Experiment, theory analysis, and numerical simulation are the three main means to investigate the microfluidic-related phenomenon and mechanism. The experiment is usually accurate, but they are often expensive. Although the theoretical analysis is cheap, it is usually not accurate enough. Numerical simulations usually achieve a trade-off between cost and accuracy.

For numerical simulation, the Lattice Boltzmann method (LBM), a flow field simulation method established and developed in the mid-1980s, has gained wide attention in recent decades. For example, LBM is used to simulate a 2D electrothermal pump [3]. The droplet-on-demand (DOD) is an important part of the microfluidic system. In [4], the authors used LBM numerical simulation to explore a low-cost Polymerase Chain Reaction based design and manufacturing method, and analyzed a flow-focused DOD system. To verify the suitability of the continuity medium hypothesis in the design of the emitter, the LBM was used to study the flow characteristics of the emitter [5]. The lattice Boltzmann method and dynamic ray tracing method are used to study the retention and coalescence behavior of microfluidic droplets under the action of an optical trap [6]. The use of two-dimensional numerical simulations with a reduced particle-based Reynolds number for studying particle migration in a microchannel with equally spaced multiple constrictions was investigated. Two-and three-dimensional colloidal lattice
Boltzmann models were used to simulate particle-fluid hydrodynamics [7].

This paper mainly reviews the application of LBM in microfluidic numerical simulation. Sec. 2 introduces the basic principles and implementation steps of LBM. LBM applications in microfluidic related particle regulation, flow control, and drug delivery are summarized in Sec. 3. Conclusion and prospects are provided in Sec. 4.

2. Background

LBM is a numerical method to simulate a flow field based on molecular motion theory and statistical mechanics. LBM is a kind of flow field simulation method established and developed in the mid-1980s. It inherits the main principle of lattice gas automata (Lattice Gas Automaton, LGA) and improves the LGA. Its particle distribution function satisfies the lattice Boltzmann (LB) equation. The LB equation can be expressed as:

\[ f_i(x + e_i \delta t, t + \delta t) - f_i(x, t) = \Omega_i(x, t) \]  

where \( f_i(x, t) \) and \( \Omega_i(x, t) \) are the particle distribution function and collision operator in the \( i \)th direction at the position \( x \) and the time \( t \), \( \delta t \) is the time step, \( e_i \) is the lattice velocity in the \( i \)th direction.

The most commonly used collision operator is:

\[ \Omega_i(x, t) = -\frac{1}{\tau_f} (f_i(x, t) - f_i^{eq}(x, t)) \]

Where \( \tau_f \) is the relaxation time, and \( f_i^{eq} \) is the equilibrium distribution function, which is defined as

\[ f_i^{eq}(x, t) = \rho(x, t) \omega_i [1 + \frac{e_i u(x, t)}{c_s^2} + \frac{1}{2} \left( \frac{e_i u(x, t)}{c_s^2} \right)^2 - \frac{1}{2} \frac{u^2(x, t)}{c_s^2}] \]

The LBM simulation includes the following steps: (1) simulates the particle's collision at that particular point with another fluid particle (2) after spread (3) apply boundary conditions (4) update time step (5) calculate the forces required (6) instantaneous update to get local density and velocity (7) particles move toward equilibrium state after a while (8) output the LBM simulation results.

![Fig.1 Flow chart of LBM simulation for a flow filed](image)

3. Application of LBM in Microfluidic Flow

In this section, typical applications of LBM in particle regulation, flow control, and drug delivery are introduced.

3.1 Particle Regulation

In [8], the effect of particle compliance on the inertial migration of microfluidic channels is investigated.
using 3d computer simulations. A hybrid calculation method is employed to simulate the dynamic interaction between elastic, submissive particles, and viscous channel flows. The LBM of viscous fluid dynamics and the lattice spring model (LSM) of elastic solid micromechanics. On the solid-fluid interface, the LBM and LSM are coupled by a non-slip boundary condition that transmits the force applied by the fluid to the solid shell, applying the local solid velocity to the surrounding viscous fluid.

They effectively captured the inertial ordering of particles observed in the experiment. The authors present a function of the dimensionless particle migration velocity and the channel wall distance. They find that the positive velocity is closer to the wall and negative closer to the midplane for all channels. The positive velocity means that the particle is away from the channel wall, where the negative velocity indicates the migration away from the plane in the channel. Therefore, there is a stable deviation from the center equilibrium position, where the particle velocity is zero.

The simulations show the following observations: (1) the larger particle equilibrium is closer to the plane in the channel. Similarly, they find that the particle equilibrium position depends on the shell compliance, and the softer particles are closer to the middle plane than the hard ones. Thus, particle deformation enhances a lift that keeps the particle away from the wall. (2) the equilibrium positions of rigid and soft particles transported by channel flow in the range of 1 to 100 do not vary with the Reynolds number of Rec channels. (3) the inertial effects in microfluidic flows can yield a useful means for sorting, focusing, and separating polymeric particles and biological cells by size, compliance, and the quality of encapsulated fluids.

In [9], the study aims to understand the effect of deformability on red blood cell (RBC) behavior of deterministic lateral displacement (DLD) devices. A model is developed and benchmarked for deformable RBCs in DLD devices to end this.

In numerical mode, the lattice-Boltzmann method (LBM) is used as fluid phase, finite element method (FEM) as membrane dynamics, immersion boundary method (IBM) as bidirectional fluid-film coupling. In order to reduce the simulation domain to a single obstacle unit, shift periodic conditions are used in the flow direction.

Simulations as following are taken:
(1) they take simulations without particles to validate the Stokes flow assumption, the bounce-base boundary condition describes the confining walls and obstacles in simulated DLD geometry.
(2) they analyze the streamline and obtain the streamline's separation distance parallel to the wall and the wall.
(3) the stretching of an RBC in an optical tweezer is simulated.

Three-dimensional high resolution immersed-boundary-lattice Boltzmann-finite-element simulations of single deformable RBCs have been performed in deterministic DLD devices. While keeping other geometric parameters fixed, they have varied the row shift d of the DLD setup, the RBC capillary number Ca, and the ratio between deforming viscous stresses and restoring the RBC membrane's elastic stresses. They showed that a deformability-based separation of RBCs in DLD devices is possible.

When the volume fraction of red blood cells becomes larger, the separation efficiency will decrease. It has the risk of flow resistance and blockage.

This study can contribute to the design of new DLD settings, deformation-based red blood cell separation, and understanding of red blood cell trajectories in such devices. This may ultimately help design cheaper, faster, and more reliable diagnostic equipment to detect malaria and other diseases. For example, It can be used to separate red blood cells from healthy red blood cells.

3.2 Flow Control

San-John An et al. [10] did a numerical study for rotating and oscillating stirrers in a microchannel. They found a new time-averaged mixing index formula to get critical values of stirring speed and maximize the efficiency under low Reynolds number (10-80). They used the LBM, as it is convenient to make adjustments to experimental boundary conditions, for example, Reynolds number and revolutions per minute for the stirrers, to evaluate the mixing rate for periodic, unsteady flows instead
of the conventional way for steady flows. D2Q9 method is used as this model has two dimensions and nine discrete velocities.

The simulation has the following results: (1). A new time-averaged mixing index with constant periods was defined as follows:

\[
D_1 = \frac{1}{T} \sum_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} \left( \frac{c_i - \bar{c}}{\bar{c}} \right)^2
\]

(4) (2). The mixing of a stationary stirrer at a lower Reynolds number is larger than that of a stationary stirrer at a large Reynolds number. (3). The mixing performance can be judged by the Peclet number 

\[Pe = \frac{v}{d} \text{Re} \]

and this vortex strength was affected by the flow speed and the stirring speed. However, the above study is based on four assumptions: 1. The flow profile is steady during the whole process. 2. Fluid’s viscosity is not affected by a change in concentration. 3. There is no friction force on the channel wall. 4. Negligible surface tension. The LBM method's simulation indicates the formula of highest stirring efficiency (different Reynolds numbers would relate to a various rotating round per minute to reach maximum rate) according to the research of this paper.

Zachary et al. [2] used computational simulations to probe the utility of actuated synthetic cilia for local regulation of the heat transport in microfluidic channels. They discovered that it could be enhanced by beating synthetic cilia. The TLBM (Thermal Lattice Boltzmann Method) is combined with the lattice spring model to simulate thermal energy transport and fluid dynamics because of the low requirement of computing power.

The TLBM model gets the overall macroscopic result by simulating collision between fluid particles in microscale, and then combine all the microscopic value to get a conclusion and analytical solution in macroscale. Two separated distribution functions of TLBM are used respectively in this model—density distribution function for microscopic fluid particles and energy distribution function for the varying temperature. A few periodic boundary conditions are also made, for example, no slipping effect and constant temperature, to simulate the regular arrangement of cilia from a single cilium.

Zachary et al. [2] calculate both steady and unsteady heat distributions under the condition of conductive and convective heat transport to validate the simulation of the TLBM method. In particular, the conductive heat transfer is modeled in rectangular domains bounded by walls with dissimilar temperatures. The convective heat transport was validated by a model in which the inlet temperatures were instantly elevated to a larger temperature at \(t=0\). The result shows that the TLBM method is valid and can reproduce numerical and analytical solutions for the system. The research shows that beating cilia, actuated by an external periodical force, can significantly enhance the heat transfer rate. Elastic filaments of cilia will be actuated and create a secondary flow due to the periodical motion. When the dimensionless sperm number is equal to 3.5, the most efficient heat transport will take place. Since the heat transfer rate depends on the parameters of cilium actuation, this method can be applied to directly regulate the local heat transport at the microscale.

### 3.3 Drug Delivery

1. Rolf Verberg et al. [11] developed a new computing method to simulate the release of nanoparticles from a microcapsule. Their aim includes two aspects: (1) model particle-filled capsules moving along a surface in a flowing fluid and the diffusion of the particles away from these carriers. (2) to determine the interactions between the released particles and an underlying substrate.

To that end, they take advantage of their two recently developed computational approaches: one for simulating the behavior of fluid-filled elastic shells, which model the capsules, and another for capturing the dynamic behavior of nanoparticle-filled fluids.

The behavior of fluid-filled elastic shells adopted their developed hybrid method, which integrates LBM for hydrodynamics and LSM for solid elastic micromechanics. Firstly, establish which LBM are connected at the solid/fluid interface. Then getting the velocities of these intersections from the adjacent
LSM nodes and next, propagating distribution functions through flowing fluid particles to their adjacent nodes, regardless of whether these nodes are in the fluid domain, otherwise, applying the appropriate boundary conditions. Finally, modify the LBM node's distribution function to consider the collision step and then repeat the whole cycle.

For the modeling of compliant capsules and surfaces, Rolf and his members simulate the system's relevant fluid-structure interactions by using the lattice Boltzmann model (LBM) and lattice spring model (LSM). They integrate the LBM for fluid dynamics and the LSM for the micromechanics of elastic solids. Brownian dynamics model (BDM) is used for the dynamics of the nanoparticles.

Their findings output a guideline of effective utilization for microcapsule carriers in the targeted delivery of nanoparticles. The Peclet number, the elasticity of the capsules, and the adhesive interaction between the capsules and the substrate all play an important role in nanoparticle deposition efficiency. Besides, their simulations revealed that the properties of the carrier capsule affected the number of adsorbed nanoparticles. The more compliant and more adhesive capsules yielded a greater number of particles at the surface. Finally, they contrasted the relative efficiency of delivering the particles via the microcapsules versus simply introducing free particles at the channel's inlet.

The future study will examine how heterogeneities within the surface can be exploited to direct the deposition of the encapsulated particles. In this manner, the particle-filled carriers could potentially be used to fill cracks in a surface and thus be harnessed to repair microscale fissures or damage on the surface of microchannels or microfluidic devices.

2. Rolf Verberg et al. [12] simulate the rolling motion of fluid-driven particle-filled microcapsules along a heterogeneous adhesive substrate to determine how the release of encapsulated nanoparticles could be used to repair the damage on the lower surface. They capture the interactions between the microcapsule's elastic shell and the surrounding fluids by using LBM for hydrodynamics and lattice spring model. The utilization of hydrophobic and hydrophilic species provides just one example of the possible chemistries that could be harnessed to produce the behavior described earlier. To actually model this complex behavior and establish the necessary design rules, we integrated the LBM, LSM, and a Brownian dynamics model. The computational efficiency of these mesoscale models allows us to capture the fluid–structure interactions in the system and the different temporal events, for example, the motion of the capsule and the convection and diffusion of the particles for the micromechanics of elastic solids. Their studies found that the following variables have a significant effect on the behavior of the system: the strength of the adhesive interaction between the capsule and the substrate. The rate of diffusion of the particles through the shell and the Peclet number of the flow. The team set up guidelines for designing particle-filled microcapsules that perform a 'repair and go' function and can be used to repair damage in microchannels and microfluidic devices.

In the future, the underlying physics that controls the behavior of this system is not dependent on the dimensionality of the system, we anticipate that we would find qualitatively similar behavior in three-dimensional systems. Studies are currently underway to extend the current model to three dimensions; since we have already employed a three-dimensional version of our integrated ‘LBM/LSM’ approach, the extension of the current model to three-dimensional can be carried out in a straightforward.

3. X. Jia and R. A. Williams [13] With the help of emerging characterization and simulation techniques, mixed models of particle structure dissolution at the microscopic scale are described in detail using real particle shapes. The hybrid approach's software implementation includes modules for particle packing, flow calculation, and dissolution simulation. A common feature shared by all modules is their digital or lattice-based approach. The lattice Boltzmann method (LBM) is used to generate flow input for convection. Their goal was to develop a computer software design assistant to help with recipe development. Their software's advantage is the straightforwardness to incorporate structural information at a microscopic (sub-particle) level, which is becoming increasingly accessible due to advances in non-destructive measurement techniques such as X-ray micro and nanotomography. However, for real and complex particle structures, further validation case studies are needed to determine, for example, how much the digitization error affects the predicted dissolution behavior. In the future, A more complex
decomposition algorithm needs to be developed to incorporate the physical and chemical mechanisms of decomposition in more detail.

4. Conclusions

LMB method is an efficient method in microfluidic related flow simulation. This paper has integrated several papers that use LBM to calculate the microfluidic motion or simulate the molecular motion. We found that the LBM has shown extraordinary potential in microfluidic computation.

In the particle regulation area, LBM helps researchers effectively captured the inertial ordering of particles. And in the flow-control area, researchers can directly regulate the local heat transport at the microscale with the LBM method. In the drug delivery area, the researchers summarized a guideline of effective utilization for microcapsule carriers in nanoparticles’ targeted delivery.

There still exist limitations for LBM in microfluidic flow simulation. For example, the LBM method is only used for two-dimensional calculations. For future study, a three-dimensional LBM method needs to be established to obtain more accurate simulation results.

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