Mesoscale Modeling of Microfluidic Flows by Lattice-Boltzmann Method

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Abstract - **In this paper the lattice Boltzmann equation approach was applied for mesoscale modeling of microfluidic multiphase flow.**

Keywords - **Mesoscale modeling, Microfluidic flow, Lattice-Boltzmann Method.**

I. INTRODUCTION

The description of biomicrofluidic flows in Lab-chip devices requires very accurate model of molecular interactions on the edge of multiphase and multicomponent systems. Classical flow models, which are based on the assumption of continuous environment, are efficient and accurate only for macroscopic scale, but they can't be unconditionally applied for micro- and nanoflows. Also, they can't be used with bio-flows, which contains biological substances, colloidal solutions and reacting polyhydric bio-molecules. These microfluidic systems rises several challenges for simulation techniques, because of presence of disparate time, length and energy scales. Atomistic models, based on quantum-mechanics, molecular dynamics and Monte Carlo methods are sufficiently accurate for the analysis of complex flows, but they required extremely high computational cost for the whole device. Thus, only generalized multiscale approach can preserve accuracy, since it provides an individual approach to each scale at different hierarchical levels, and provides a realistic simulation of the whole microfluidic system [1].

Modern fast and parallel CAD/CAE simulation tools could solve various complex and nonlinear multiphysical problems directly, without using any prior mathematical simplifications or approximations. Hence, the majority of research activities in the field of multiscale modeling and simulation is based on the new class of numerical and analytical modeling techniques. One can point out three main approaches for solving the multiscale modeling [2]:

- Methods of multiscale discretization, that allow different scales (levels) within a single system model and dynamically adjust the dividing ability, depending on space, time and data;
- Hybrid methods that combine several different models and types of numerical representations that describes different scales (levels);
- Methods that provide analytical representations for different effects at lower levels, and are used in numerical modeling at higher levels.

II. MESOSCALE LEVEL IN FLUID FLOW MODELING

Very often microfluidic flows deals with complex mixtures, colloidal suspensions, bio-solutions with complex biochemical reactions (combustion), including the influences of self-moving bio-objects and rheological behavior of cell clusters. All these systems has one joint phenomena: the microfluidic flow completely depends upon mesoscopic length-scales effects. The mesoscale level includes the lengths and times, which lay down between micro- and macro- scales. It helps to fill the gap between continuum and discrete (atomistic) levels. This region is not mandatory, and for ideal or simple fluids it can be simply ignored and excluded from simulation procedures. Its dimension is smaller than regular continuum scale, but larger than the discreet atomistic scale. The time scale of mesoscale level generally cover the period from 0,1 μs up to 1,0 μs.

Current activity in the field of mesoscale modeling and simulations is based on a new class of numerical and analytical modeling techniques. These new techniques promise to be more effective than traditional multigrid or multiresolution methods that were designed to deal with small-scale problems in the entire macroscopic region. Recently, several atomistic simulation methods were developed, namely - Dissipative Particle Dynamics (DPD), Molecular Dynamics (MD), Lattice-Boltzmann Equation (LBE) and Direct Simulation Monte Carlo (DSMC). The common idea of all these techniques consist in local averaging of bio-fluidic microscopic parameters within the real physical processes in order to achieve high computational efficiency. Each atomistic method is sufficiently accurate for the analysis of complex meso-and microflows. However, the extremely high computational cost suppress its application for the entire device. In this case, only generalized multiscale modeling, which uses the hybrid finite element method, allows us to keep accuracy, as it provides individual attention in an appropriate scale and hierarchical levels.

It is known, that there are two main approaches for fluidic flow modeling at mesoscale level:

1. hybrid approach, which combines molecular and continuum approach;
2. simplification approach, which allow to formulate mesoscale model from the molecular by some transformations.

Here we consider hybrid approach, because it can be easily implemented in combination with existed continuum and newly developed atomistic models. The

examples of successful applications of hybrid approach described in [3].

At hybrid approach, atomistic models usually applied near the surfaces and phase interfaces, and continuum models - in the bulk region [4]. It is very difficult to define the overlapped domain in this case, and hard to formulate the proper boundary conditions between molecular and continuum regions. Hence, such inner-boundaries introduces additional error to the model, which is very difficult to estimate. Besides, the time scales for continuum and atomistic approaches do not match and requires coordination. Thus, the general mesoscale simulation procedure appointed to calculate main mesoscale parameters from the molecular approach and to pass them to the continuum simulation. This provide relative independence: simulation procedures run independently and occasionally communicate between themselves.

III. Coupling between scales

Communication between the atomistic and continuum levels is a challenge due to the nature of the information, being calculated at each scale [5].

- at continuum scale such parameters, as velocities and pressure are relatively smooth functions of spatial and temporal variables with minimum stochastic influence (turbulent conditions excluded in microfluidic devices).
- at discrete (atomistic) scale, microfluidic parameters can be calculated by averaging of dynamic variables in order to connect them with a thermodynamic continuum variable such as temperature and pressure.

The general coupling algorithm, which is based on hybrid finite-element method, is shown in fig.1.

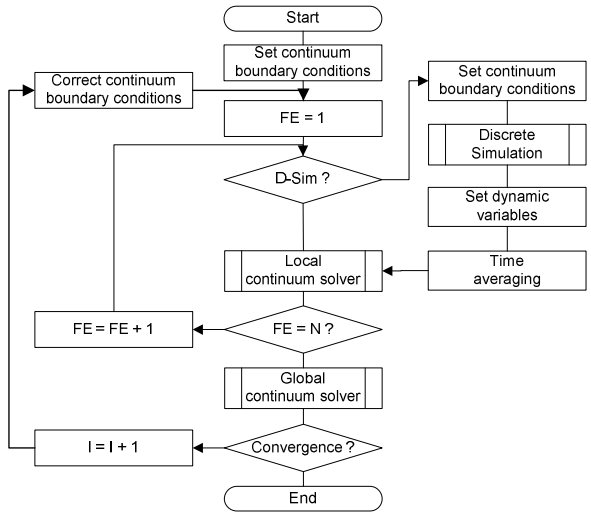


Fig.1. Algorithm of sequential coupling between continuum and atomistic models.

At first step, the atomistic modeling information should be entered from the literature sources, but in the next steps it will be obtained from concurrent simulations.

In the mentioned sequential coupling the atomistic simulation is performed with the preset boundary conditions, in order to extract information or a reduced model. The continuum scale variables are then calculated by using time averaging and statistical techniques in order to produce a modified boundary condition for the continuum simulation.

IV. Lattice Boltzmann Equation Method

The most promised alternative for CFD simulation is lattice Boltzmann equation method (LBE), where fluid is treated as fictitious mesoscopic particles (not molecules). Basically, it uses the special version of Boltzmann equation, which describes the particles interaction on fixed lattices and just simulates the flow of Newtonian fluid. Although LBE can be expanded to completely replace the Navier-Stokes equations in modeling the incompressible and compressible microfluidic flows, the application of LBE in actual work is typical mesoscale. As a mesoscale method, it connects the microscopic and macroscopic descriptions of the flow dynamics. Such macroscopic parameters, as density (ρ) and velocity (v) can be easily calculated as soon as LBE solution will be obtained. This has significant advantages in some microfluidic areas, connected with multicomponent and multiphase biofluidic flows.

Computer modeling of phase transformations can be implemented in LBE method through calculation of phase boundaries, emerging in the bulk microfluidic mixture. To describe the equation of state, allowing phase transitions, it was necessary to introduce forces acted on the mixture in the neighboring nodes. These forces also provide the surface tension at the interface between different phases.

It was underlined, that the physics of microfluidics flow and fluid properties can be accurately incorporated into the LBE method, even more accurate than in Navier-Stokes equations [6]. Consequently, the proposed mesoscopic modeling approach, based upon LBE method, is particularly suitable for surface and interfacial phenomena [7], multiphase bioflows [8], porous media flows [9], and others, that are typical in microfluidics.

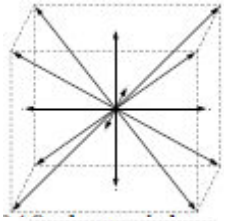
In the LBE method, a particle distribution function f(x, t) is solved as a function of time t and space x. The space is represented by lattices at fixed positions. Hence, the computer application of LBE includes collision (1) and streaming (2) steps:

$$\begin{cases} f_i^t\left(\vec{x}, t+\delta_t\right) = f_i\left(\vec{x}, t\right) + \dfrac{1}{\tau_f}\left(f_i^{eq} - f_i\right) & (1) \\ f_i\left(\vec{x}+\vec{e}_i\delta_t, t+\delta_t\right) = f_i^t\left(\vec{x}, t+\delta_t\right) & (2) \end{cases}$$

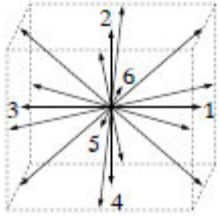
where *i* are the directions of momentum.

Here the velocity is discretized in a space to a finite number of vectors v_i, space to a lattice where it requires that $(x+v_i)$ is again a lattice position and time only takes on integer values. For LBE implementation one can use a number of different lattice models - cubic or triangular, and with or without the rest particles in the discrete distribution function. For 3D calculations the

fifteen (D3Q15) and nineteen(D3Q19) speed variant of the LBE model is often used [10]:



$$w_i = \begin{cases} 2/9 & i = 0 \\ 1/9 & i = 1-6 \\ 1/72 & i = 7-14 \end{cases}$$



$$w_i = \begin{cases} 1/3 & i = 0 \\ 1/18 & i = 1-6 \\ 1/36 & i = 7-18 \end{cases}$$

The accuracy of LBE method depends on: 1) physical problem; 2) numerical implementation; 3) used models/correlation. The LBE method can't guarantee any accurate results - it depends upon the software implementation, and the user application.

V. Parallel computing on GPUs

Graphics processor units on modern video cards (GPU) have unique ability to parallel computing on a large number of GPU cores, based on CUDA technology. As far as LBE algorithm runs computation mostly in the local node, except for the particles transport and gradient calculation, which takes into account neighboring nodes, it allows to parallelize calculations on a large number of GPU cores [11].

Parallel calculations were performed on the graphics card from NVIDIA [12]. LBE algorithm involves computation primarily in the local nodes of the computational grid, except for the particles transport and interaction forces of between nodes. Thus, it allows to parallelize a large number of elementary calculations [13]. To parallelize the algorithm on a large number of GPU cores the CUDA programming technology was used.

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III. Conclusion

In actual research it was shown, that mesoscale simulation, which is based on real-time coupling between the continuum and atomistic level can significantly help in accurate microfluidic device design. LBE method provides an effective approach for modeling multiphase Lab-chips flows.

Several, most obvious advantages of LBE method includes: 1) Intrinsic linear scalability in parallel computing that can be efficiently solved, because the collision are calculated locally; 2) Easy dealing with arbitrarily complex geometries: geometric complexity of microfluidic channels is not a challenge, because of the simple solid moving and domain deformation; 3) Efficient inter-phase interaction handling for multiphase flow because phase interaction is inherently included in the particle collisions.

Acknowledgements

Results presented in the paper are supported by Marie Curie International Research Staff Exchange Scheme Fellowship within the 7th European Community Framework Programme - - EduMEMS - Developing Multidomain MEMS Models for Educational Purposes, no. 269295.