The Lattice Boltzmann Method for Two-Phase Flows and Applications to Filtration Processes

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Abstract. In the lattice Boltzmann method (LBM), macroscopic flow behavior is described by simulating a very simple, fully discrete, microscopic gas model instead of discretizing the flow equations directly. Based on the frequently used D2Q9 model (nine discrete velocities in two space dimensions), we show how surface tension effects can be combined with LBM. The applicability of the two-phase lattice Boltzmann method is demonstrated with simulations of filtration processes.

1 Introduction

In lattice Boltzmann methods, discrete velocity models of kinetic equations are used to obtain approximate solutions of the incompressible Stokes or Navier-Stokes system. The idea of LBM rests on the observation that the kinetic and the macroscopic models are equivalent in the limit of small Knudsen and Mach numbers (see [1,4,5,13] for reviews on LBM). Extensions of the method to two phase flows, so called immiscible lattice Boltzmann models, originate in lattice gas cellular automata [6,7,11,12]. While most of these approaches are based on hexagonal grids with seven kinetic velocities, we present a generalization which is applicable to all lattice Boltzmann schemes in two and three dimensions and with arbitrary numbers of velocities.

A general advantage of lattice Boltzmann schemes is the easy applicability to flows in complex geometries, for example, the flow of an air-oil mixture through a filter (i.e. a combination of porous materials). The basic goal in the design of such filters is the maximization of oil absorption with the side condition that the pressure drop, which is related to the energy consumption of the process, is as small as possible. The macroscopic flow through the filter can be approximated by a two-phase Darcy's law but this approach requires material parameters such as relative permeabilities. Since the experimental determination of these dynamical properties is a difficult task, a natural idea is to resort to numerical simulations. To this end, a representative element of the filter (a periodicity cell) is considered (see Fig. 1). The fiber structure of the filter is generated stochastically and is controlled by anisotropy parameters and a prescribed radius distribution to model different filter materials. The flow of the oil-gas mixture is characterized by a small Reynolds number ($Re \approx 0.01$) and can be described by the two-phase Stokes equation. The ratio of dynamic viscosities is $\mu_{oil}/\mu_{gas} \approx 1000$.

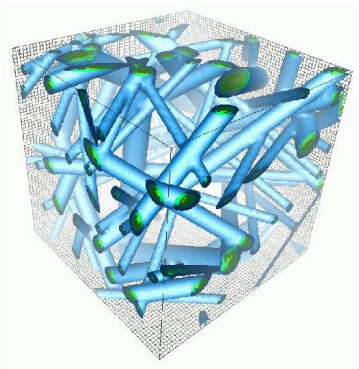

Fig. 1. Periodicity cell of the filter material

The discretization with the Lattice Boltzmann method is carried out by superposing the geometry with a regular cubic mesh in which all mesh points are deleted which are located in the fiber material. On the remaining mesh points, the simple lattice Boltzmann evolution is carried out consisting of transport and collision steps and so called recoloring steps which are required to keep the phases separated. Typical results are given in Fig. 2 which show the interfaces between oil and air and the fibers of the filter. While the left figure represents an isotropic distribution of fibers, the anisotropy in the right one is much stronger. Here, the fibers are almost aligned in vertical direction.

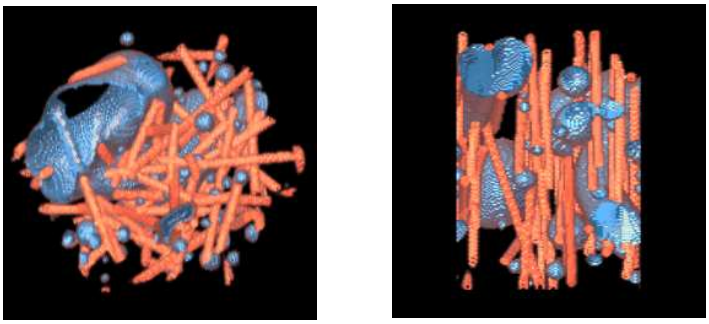

Fig. 2. Oil interface in a filter structure

2 The Two-Phase Stokes Equation

We assume that the two phases occupy the sets $\Omega_1(t), \Omega_2(t)$ in $\mathbb{R}^d$, $d \in \{2, 3\}$ with the common interface $\Gamma(t)$. The regular interface has a field $\boldsymbol{n}$ of unit

normal vectors and moves with the flow velocity $\boldsymbol{u}$ which is, in each phase, a solution of the Stokes equation

$$\frac{\partial \boldsymbol{u}}{\partial t} = \frac{1}{\varrho} \operatorname{div} \sigma, \qquad \operatorname{div} \boldsymbol{u} = 0, \qquad \boldsymbol{x} \in \Omega_i,\ i = 1, 2. \tag{1}$$

Here, $\sigma_{ij} = -p\delta_{ij} + 2\mu S_{ij}$ is the stress tensor with pressure p and viscous stresses $S_{ij} = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2$ which are proportional to the fluid viscosity μ. At the fluid interface Γ, the surface tension balances the jump of the normal stresses. Together with the assumed continuity of $\boldsymbol{u}$, this leads to the conditions $[\boldsymbol{u}] = \boldsymbol{0}$, and $[\sigma \boldsymbol{n}] = \alpha\kappa\boldsymbol{n}$, where α is a (constant) surface tension coefficient, κ is the mean curvature of Γ and $[\cdot]$ denotes the difference on the interface between limits from the two phases.

For our purpose, it is convenient to transform the Stokes equations (1) in each phase together with the jump condition into a single equation on the full space $\mathbb{R}^d$. This idea is frequently used in the simulation of multi-phase flows (see, for example, [3,2] and the references therein). We first bring (1) in a weak form by multiplying the equations with a test function and integrating by parts. Then, we add the resulting expressions, take the jump conditions into account and introduce $\langle \delta_\Gamma, \phi \rangle := \int_\Gamma \phi \, do$ as a surface distribution. Eventually, we obtain the two-phase Stokes equation on the full space $\mathbb{R}^d$ but now in a distributional sense

$$\frac{\partial \varrho \boldsymbol{u}}{\partial t} = \operatorname{div} \sigma - \alpha\kappa\boldsymbol{n}\delta_\Gamma, \qquad \operatorname{div} \boldsymbol{u} = 0. \tag{2}$$

It has been noted in [10] that the surface tension term $\kappa\boldsymbol{n}\delta_\Gamma$ can be written as a divergence $\kappa\boldsymbol{n}\delta_\Gamma = \operatorname{div}((I - \boldsymbol{n} \otimes \boldsymbol{n})\delta_\Gamma)$, where I is the identity matrix. This allows us to reformulate (2) as

$$\frac{\partial \varrho \boldsymbol{u}}{\partial t} + \operatorname{div}(\alpha(I - \boldsymbol{n} \otimes \boldsymbol{n})\delta_\Gamma) = \operatorname{div} \sigma, \qquad \operatorname{div} \boldsymbol{u} = 0. \tag{3}$$

Written in this way, the two-phase Stokes equation appears formally like the single-phase Navier-Stokes equation if we replace the surface tension term by the inertia term $\varrho\boldsymbol{u} \otimes \boldsymbol{u}$. This simple observation turns out to be very useful to construct a lattice Boltzmann approximation of (3). The correct dynamical behavior is obtained by replacing $\varrho\boldsymbol{u} \otimes \boldsymbol{u}$ in the single-phase Navier-Stokes lattice Boltzmann algorithm with the expression $\alpha(I - \boldsymbol{n} \otimes \boldsymbol{n})\delta_\Gamma$. Of course additional care has to be taken to represent δ_Γ and to keep the two fluids separated.

3 LBM for the Navier-Stokes Equation

To understand the lattice Boltzmann algorithm, one can think of a hypothetical liquid whose atoms can only stay at discrete nodes of a regular lattice.

Here, we consider the case of a square lattice in two space dimensions. In each discrete time step, the atoms either rest at their node or move to a neighboring site. In the case of a square grid, this gives rise to nine possible velocities $\boldsymbol{C}_0, \ldots, \boldsymbol{C}_8 \in \{-1, 0, 1\}^2$. Consequently, the state of the liquid is completely described if the densities N_i of atoms with velocities $\boldsymbol{C}_i$ are known at each node. Macroscopic quantities like the total mass density ρ or the average velocity $\boldsymbol{u}$ are then given as averages of the microscopic densities $\rho = \sum_i N_i$ and $\boldsymbol{u} = \sum_i N_i \boldsymbol{C}_i / \rho$. The state evolution of this hypothetical liquid now consists of two steps: in the collision phase, atoms arriving from neighboring nodes interact instantaneously and may change their velocities which leads to a local redistribution of the densities N_i in which total mass and momentum are conserved. The tendency in this interaction is towards an equilibrium distribution

$$N_i^{eq} = N_i^* \left(\rho + 3\rho \boldsymbol{u} \cdot \boldsymbol{C}_i + \frac{9}{2} \rho \boldsymbol{u} \otimes \boldsymbol{u} : (\boldsymbol{C}_i \otimes \boldsymbol{C}_i - I/3) \right) \tag{4}$$

where N_i^* are constants (4/9 for the zero velocity, 1/9 for the velocities of length one, and 1/36 for those of length $\sqrt{2}$), $\boldsymbol{u} \otimes \boldsymbol{u}$ is a matrix with entries $u_i u_j$ and the colon denotes the matrix scalar product $A : B = \sum_{i,j} A_{ij} B_{ij}$. We remark that equilibrium distributions for other lattices have the same structure and differ only in the constants.

After collision, the atoms move in a discrete time step to neighboring sites. The combination of the two steps leads to the evolution

$$N_i(t+1, \boldsymbol{x} + \boldsymbol{C}_i) = N_i(t, \boldsymbol{x}) + \omega (N_i^{eq}(t, \boldsymbol{x}) - N_i(t, \boldsymbol{x}))$$

If the average velocity $\boldsymbol{u}$ in this process is small compared to the microscopic velocities, one obtains an approximate Navier-Stokes solution where the variations in the density are related to the pressure and the viscosity is controlled by ω. Usually, this behavior is explained by performing a Chapman-Enskog expansion [13] but it also follows from a simple transformation of variables [8].

4 LBM for the Two-Phase Stokes Equation

To obtain a lattice Boltzmann algorithm for the two-phase Stokes equation, we modify the algorithm of the previous section by replacing $\rho \boldsymbol{u} \otimes \boldsymbol{u}$ in (4) with an approximation of $\alpha(I - \boldsymbol{n} \otimes \boldsymbol{n})\delta_\Gamma$. In the standard immiscible lattice Boltzmann algorithm [7], the approximation is obtained from the macroscopic mass densities ρ_1 and ρ_2 of the fluids occupying Ω_1 and Ω_2. The difference $\chi = \rho_1 - \rho_2$ is positive in Ω_1 and negative in Ω_2. Hence, if ρ_i are smooth functions which quickly decay to zero in a narrow mixing region, we can define the interface as the level set $\{\chi = 0\}$. The normal field is then obtained by $\boldsymbol{n} = \nabla\chi / |\nabla\chi|$ and since χ approximates a jump function, the surface

delta distribution δ_Γ satisfies $\delta_\Gamma \approx c|\nabla\chi|$ where c is the inverse of the jump height. The gradient of χ is typically discretized by an expression of the form $\boldsymbol{F} = \sum_i \boldsymbol{C}_i \chi(\boldsymbol{x} + \boldsymbol{C}_i)/6$ which is called *color gradient*. Note that this is just a compact way of denoting the finite difference stencils

$$F_1 = \frac{1}{6}\begin{bmatrix} -1 & 0 & 1 \\ -1 & 0 & 1 \\ -1 & 0 & 1 \end{bmatrix}\chi, \qquad F_2 = \frac{1}{6}\begin{bmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \end{bmatrix}\chi$$

which clearly approximate the gradient. Combining these steps, we arrive at the approximation

$$(I - \boldsymbol{n} \otimes \boldsymbol{n})\delta_\Gamma \approx (I - \boldsymbol{F} \otimes \boldsymbol{F}/|\boldsymbol{F}|^2)|\boldsymbol{F}|.$$

Finally, a mechanism is required to transport the interface along with the flow which prevents the mixing of the two liquids. In the classical immiscible lattice Boltzmann algorithm, the densities ρ_1 and ρ_2 are related to microscopic distributions $N_i^{(1)}$ and $N_i^{(2)}$ whose sum N_i is the total distribution which appears in the main algorithm. If the transport step in this algorithm is implemented as a separate transport of $N_i^{(1)}$ and $N_i^{(2)}$, one can show that the resulting evolution of $\chi = \rho_1 - \rho_2$ is consistent to an advection diffusion equation [9]. To counteract the unwanted diffusion which is related to a flux proportional to $-\nabla\chi$, the so called *recoloring step* is used. In this step, the distributions $N_i^{(j)}$ are modified in such a way that the vector $\boldsymbol{w} = \sum_i (N_i^{(1)} - N_i^{(2)})\boldsymbol{C}_i$, which controls the flux of $\chi = \sum_i (N_i^{(1)} - N_i^{(2)})$ due to transport, points preferably opposite to $-\nabla\chi$. More precisely, the scalar product $\boldsymbol{w} \cdot \boldsymbol{F}$ is maximized under side conditions which ensure nonnegativity of distributions and conservation of total mass and momentum. This approach leads to an efficient transport method for χ which maintains a sharp interface (a more detailed investigation can be found in [9]).

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