A multiphase lattice Boltzmann model with sharp interfaces

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Introduction

Multiphase lattice Boltzmann models usually fall into one of three categories: Colour gradient, or Rothman-Keller, models; Shan-Chen models; or free-energy models. The Free-Energy and Shan-Chen models are intended to simulate flows where the kinematics of phase separation or interactions at the molecular level are of interest. These models do not allow for independent adjustment of either the surface tension or the viscosity ratio and the resolved interface is spread over several lattice nodes. Here we are concerned with macroscopic, immiscible, flows and therefore pursue colour-based models since they offer the most attractive features to the modeller who wishes to simulate binary flows on the length scale addressed by continuum mechanics.

We introduce a phase field (or colour field) ϕ to represent the different fluids. Regions where the phase field $\phi \approx 0$ might represent one phase (e.g oil) and regions where $\phi \approx 1$ the other phase (e.g water). In principle, ϕ is advected by the fluid velocity, hence $\phi_t + \mathbf{u} \cdot \nabla \phi = 0$. However, to make the most of limited spacial resolution it is common to add a "sharpening term" to counteract the inevitable numerical diffusion and preserve relatively thin boundaries between different phases. For example, the sharpening term might drive all points where $\phi > \frac{1}{2}$ back towards $\phi = 1$, and all points where $\phi < \frac{1}{2}$ back towards $\phi = 0$. The width of the phase boundary is then controlled by a balance between diffusion and the sharpening term. However, overly narrow phase boundaries can fail to propagate correctly, becoming fixed or "pinned" to the grid [1].

Phase field sharpening and pinning

A useful model for studying hyperbolic equations with "stiff" source terms is [2]:

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = S(\phi) = -\frac{1}{T}\phi\,(1-\phi)\,(\phi_c - \phi),$$

The problem is called stiff when the timescale T of the source term is much shorter than a typical advective timescale.

Using an over-long timestep may cause plausible but spurious numerical behaviour:

"The numerical results presented above indicate a disturbing feature of this problem – it is possible to compute perfectly reasonable results that are stable and free from oscillations and yet are completely incorrect. Needless to say, this can be misleading." [2]

This sounds exactly like pinning.

Random projection method

A deterministic value of ϕ_c causes the phase field to become "pinned" to the lattice. However, taking ϕ_c to be a quasi-random variable chosen from a van der Corput sampling sequence [3] greatly reduces this spurious phenomenon [4].

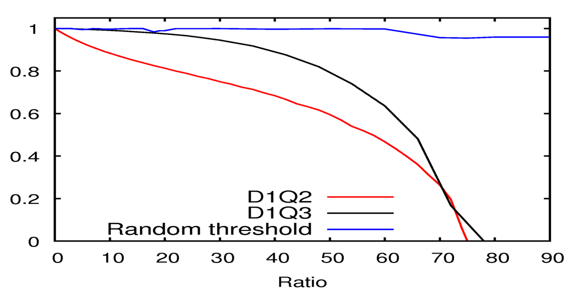

Fig. 1: Interface propagation speeds as a function of τ/T.

Multiphase LBM

We introduce two discrete Boltzmann equations with distribution functions f_i and g_i for the fluid flow and phase field, respectively:

$$\begin{aligned}\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i &= -\frac{1}{\tau_f}\left(f_i - f_i^{(e)}\right);\\ \frac{\partial g_i}{\partial t} + \mathbf{c}_i \cdot \nabla g_i &= -\frac{1}{\tau_g}\left(g_i - g_i^{(e)}\right) + R_i,\end{aligned}$$

where

$$\begin{aligned} f_i^{(e)} &= W_i\rho\,(1 + 3\mathbf{c}_i\cdot\mathbf{u} + \\ &\quad \frac{9}{2}\left(\mathbf{uu} + \sigma\mathbf{I}\left(\frac{1}{3}(|\mathbf{c}_i|^2 + |\mathbf{n}|^2) - (\mathbf{c}_i\cdot\mathbf{n})^2\right)\right) : (\mathbf{c}_i\mathbf{c}_i - \frac{1}{3}\mathbf{I})\Big),\\ g_i^{(e)} &= W_i\phi\,(1 + 3\mathbf{c}_i\cdot\mathbf{u}),\\ R_i &= -W_i S(\phi)\,(1 + 3\mathbf{c}_i\cdot\mathbf{u}).\end{aligned}$$

Here, $\rho = \sum_i f_i$, $\rho\mathbf{u} = \sum_i f_i\mathbf{c}_i$, $\phi = \sum_i g_i$, $S(\phi) = \sum R_i$, σ is the surface tension and $\mathbf{n} = \nabla\phi/|\nabla\phi|$ is the interface unit normal, which is approximated using central differences. The surface tension is included directly into the equilibrium distribution.

Macroscopic equations

Applying the Chapman-Enskog expansion to the fluid equation yields

$$\begin{aligned}\frac{\partial \rho}{\partial t} &+ \nabla\cdot\rho\mathbf{u} = 0,\\ \frac{\partial \rho\mathbf{u}}{\partial t} &+ \nabla\cdot(P\mathbf{I} + \rho\mathbf{uu}) = \nabla\cdot\left(\mu\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^\dagger\right)\right)\\ &+\sigma\nabla\cdot(\mathbf{I} - \mathbf{nn})\,\delta_s + O(Ma^3),\end{aligned}$$

where $\mu = \tau_f\rho/3$ is the dynamic viscosity and δ_s is the surface delta function. In the small Mach number limit, these are the continuous surface force equations of Brackbill *et al.* [5]. Note that the surface tension coefficient in the macroscopic equations is precisely σ from the discrete Boltzmann equation.

Applying the Chapman-Enskog expansion to the phase field equation yields

$$\frac{\partial \phi}{\partial t} + \nabla\cdot(\phi\mathbf{u}) = S(\phi) + \tau_g\left(\frac{1}{3}\mathbf{I} - \mathbf{uu}\right) : \nabla\nabla\phi + O(\tau_g^2).$$

To leading order this is the sharpening equation with an additional $O(\tau_g)$ diffusive term, which sets the width of the interface.

Fully discrete form

The previous two discrete Boltzmann equations can be discretised in space and time by integrating along their characteristics to obtain a second-order algorithm:

$$\begin{aligned}\overline{f}_i(\mathbf{x} + \mathbf{c}_i\Delta t, t+\Delta t) - \overline{f}_i(\mathbf{x}, t) &= -\frac{\Delta t}{\tau_f + \Delta t/2}\left(\overline{f}_i(\mathbf{x},t) - f_i^{(e)}(\mathbf{x},t)\right),\\ \overline{g}_i(\mathbf{x} + \mathbf{c}_i\Delta t, t+\Delta t) - \overline{g}_i(\mathbf{x}, t) &= -\frac{\Delta t}{\tau_g + \Delta t/2}\left(\overline{g}_i(\mathbf{x},t) - g_i^{(e)}(\mathbf{x},t)\right)\\ &\quad + \frac{\tau_g\Delta t}{\tau + \Delta t/2}R_i(\mathbf{x},t),\end{aligned}$$

where the following change of variable has been used to obtain an explicit second order system at time $t + \Delta t$:

$$\begin{aligned}\overline{f}_i(\mathbf{x},t) &= f_i(\mathbf{x},t) + \frac{\Delta t}{2\tau_f}\left(f_i(\mathbf{x},t) - f_i^{(e)}(\mathbf{x},t)\right),\\ \overline{g}_i(\mathbf{x},t) &= g_i(\mathbf{x},t) + \frac{\Delta t}{2\tau_g}\left(g_i(\mathbf{x},t) - g_i^{(e)}(\mathbf{x},t)\right) - \frac{\Delta t}{2}R_i(\mathbf{x},t).\end{aligned}$$

However, we need to find ϕ in order to compute $f_i^{(0)}$ and R_i.

Reconstruction of ϕ

The source term does not conserve ϕ:

$$\begin{aligned}\bar{\phi} = \sum_i \overline{g}_i &= \sum_i\left[g_i - \frac{\Delta t}{2\tau}\left(g_i - g_i^{(e)}\right) - \frac{\Delta t}{2}R_i\right]\\ &= \phi + \frac{\Delta t}{2T}\phi\,(1-\phi)\,(\phi_c - \phi) = N(\phi).\end{aligned}$$

We can reconstruct ϕ by solving the nonlinear equation $N(\phi) = \bar{\phi}$ using Newton's method:

$$\phi \to \phi - \frac{N(\phi) - \bar{\phi}}{N'(\phi)}.$$

For the random projection case, we must convert from $\overline{g}_i$ to the g_i using the threshold from the previous timestep, $\phi_c^{(n-1)}$, and then from g_i to the $\overline{g}_i$ using the current threshold $\phi_c^{(n)}$.

Numerical Results

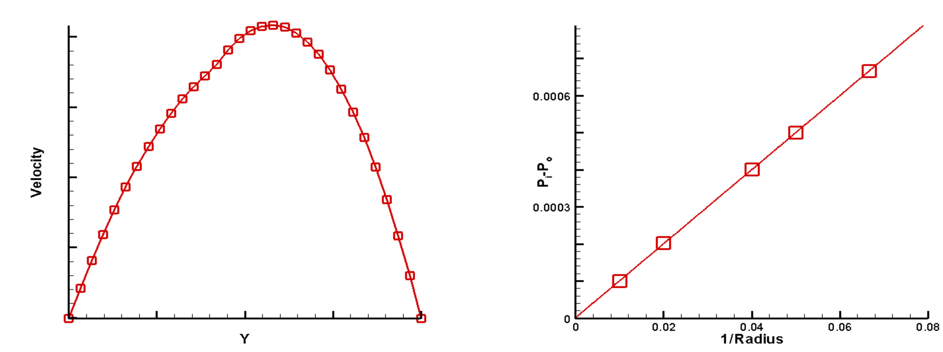

Fig. 2: Numerical validation of the proposed model.
Left: Numerical validation of layered Poiseuille flow. The symbols are the numerical predictions and the solid line is the analytic solution.
Right: Laplace's law. The symbols are the numerical predictions. The slope of the curve is σ.

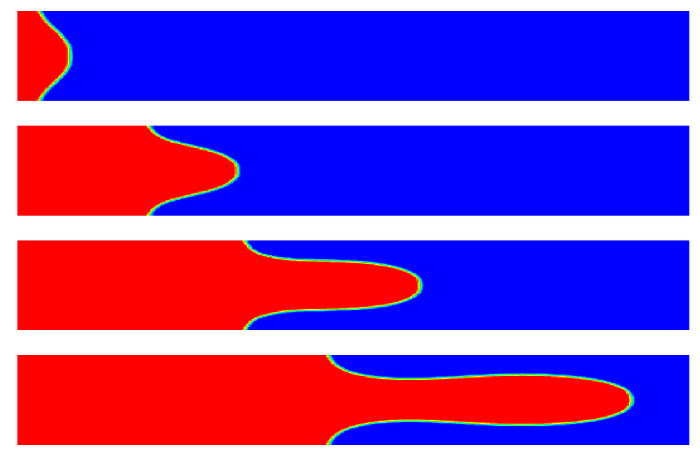

Fig. 3: Numerical simulation of viscous fingering. Here the capillary number is $Ca = 0.1$ and the viscosity ratio is 20. The interface thickness is less than 3 grid cells.

Conclusions

We have presented a continuum-based multiphase lattice Boltzmann method where the surface tension is included directly into the momentum flux tensor, eliminating the need for an additional "body force" obtained though spatial derivatives of a source term. This removes the viscosity-dependence from the surface tension which would otherwise appear due to the second-order moments in the Chapman-Enskog expansion. Separation of phases is maintained by an additional equation for the advection and sharpening of a phase field [4].

The numerical scheme is validated against the analytical solution of layered Poiseuille flow. Preliminary investigations of viscous fingering confirm the method's ability to maintain sharp interfaces, free from lattice pinning. Moreover, verification of Laplace's law confirms that the parameter σ is precisely the value of the surface tension.

References

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