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Hybrid lattice Boltzmann model for binary fluid mixtures

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Outlook

- Thermo-hydrodynamics for binary fluid mixtures
  - The equilibrium free energy
  - The macroscopic equations
    - The Navier-Stokes (NS) equation
    - The convection-diffusion (CD) equation

- Hybrid lattice Boltzmann model
  - The lattice Boltzmann equation (LBE)
  - LBE with forcing term for the NS equation
  - Continuum limit
  - Numerical scheme for the CD equation

- Numerical validation
  - Relaxation to equilibrium
  - Spurious velocities

- Conclusions and Perspectives

Equilibrium thermodynamics

The equilibrium is described by a free energy

$$\mathcal{F}[n,\phi] = \int d\mathbf{r} \left[nT \ln n + \frac{a}{2}\phi^2 + \frac{b}{4}\phi^4 + \frac{\kappa}{2}(\nabla\phi)^2 \right]$$

n is the total density
T is the temperature (assumed constant)
ϕ is the concentration difference

- The first term gives the ideal gas pressure $p^i = nT$
- The polynomial terms in ϕ describe the bulk properties of an ordered mixture ($a < 0, b > 0$) with equilibrium values $\pm\phi_{eq}$ with $\phi_{eq} = \sqrt{-a/b}$
- The last term ($\kappa > 0$) controls the interface between the two components

The equilibrium profile between the two components is

$$\phi(x) = \sqrt{\frac{-a}{b}} \tanh\left(\frac{2x}{\xi}\right)$$

with interface width

$$\xi = 2\sqrt{-2\kappa/a}$$

The thermodynamic functions can be obtained from the free energy:

- The chemical potential difference between the two components is

$$\mu = \frac{\delta \mathcal{F}}{\delta \phi} = a\phi + b\phi^3 - \kappa \nabla^2 \phi$$

- The pressure $P_{\alpha\beta}$ is a tensor since interfaces in the fluid can exert nonisotropic forces. The diagonal part p_0 read as

$$p_0 = p^i + \frac{a}{2}\phi^2 + \frac{3b}{4}\phi^4 - \kappa\phi(\nabla^2\phi) - \frac{\kappa}{2}(\nabla\phi)^2$$

The final form for the pressure tensor is

$$P_{\alpha\beta} = p_0 \delta_{\alpha\beta} + \kappa \partial_\alpha \phi \partial_\beta \phi$$

which ensures the equilibrium condition $\partial_\alpha P_{\alpha\beta} = 0$

The macroscopic equations

At constant temperature the continuum equations are

- The continuity equation

$$\partial_t n + \partial_\alpha (n u_\alpha) = 0$$

- The Navier-Stokes (NS) equation (written in $2d$)

$$\partial_t (n u_\beta) + \partial_\alpha (n u_\alpha u_\beta) = -\partial_\alpha P_{\alpha\beta} +$$

$$+\partial_\alpha \left[\eta(\partial_\alpha u_\beta + \partial_\beta u_\alpha - \delta_{\alpha\beta}\partial_\gamma u_\gamma) + \zeta \delta_{\alpha\beta}\partial_\gamma u_\gamma\right]$$

  u is the fluid velocity
  η and ζ are the shear and bulk viscosities

- The convection-diffusion (CD) equation

$$\partial_t \phi + \partial_\alpha (\phi u_\alpha) = \Gamma \nabla^2 \mu$$

  Γ is a mobility coefficient

The lattice Boltzmann equation (LBE)

The distribution functions of the fluid particles $f_i(\mathbf{r},t)$, residing on the link i of the lattice site $\mathbf{r}$ at the discrete time t, are updated according to the rule

$$f_i(\mathbf{r}+\mathbf{e}_i\Delta t, t+\Delta t) - f_i(\mathbf{r},t) = -\frac{\Delta t}{\tau}[f_i(\mathbf{r},t) - f_i^{eq}(\mathbf{r},t)]$$

τ is a relaxation parameter
$\mathbf{e}_i$ are lattice velocity vectors ($|\mathbf{e}_i| = 0, c, \sqrt{2}c$)
$f_i^{eq}(\mathbf{r},t)$ are the equilibrium distribution functions

- The density n and the momentum $n\mathbf{u}$ are given by

$$n = \sum_i f_i \qquad n\mathbf{u} = \sum_i f_i \mathbf{e}_i$$

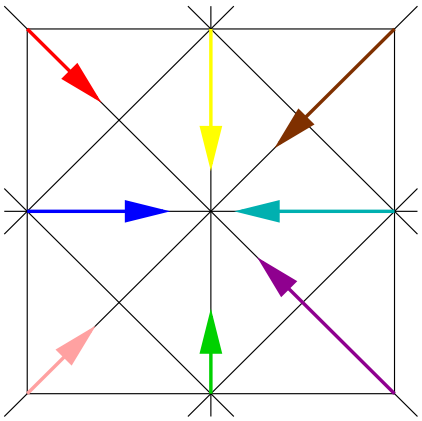
- f_i^{eq} are chosen to conserve locally density and momentum and are given by a second order expansion in the fluid velocity u of the Maxwell-Boltzmann distribution

In a previous model based on a free energy (Yeomans model) the second moment of f_i^{eq} was modified to describe binary fluid mixtures

The time evolution occurs in two steps

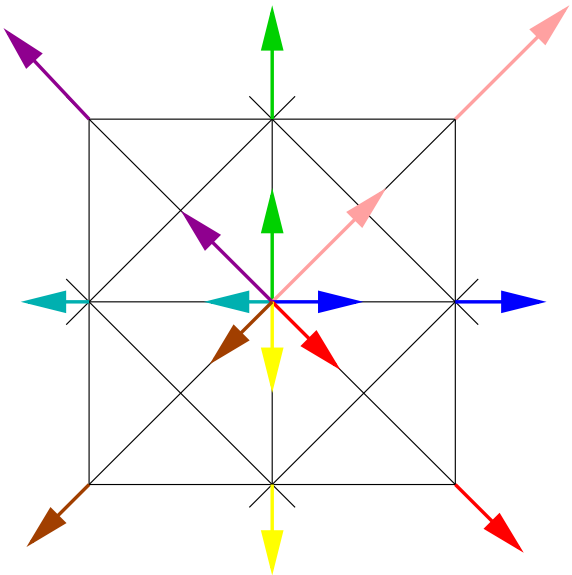
- Collision

$$f_i^c(\mathbf{r},t) = f_i(\mathbf{r},t) - \frac{\Delta t}{\tau}[f_i(\mathbf{r},t) - f_i^{eq}(\mathbf{r},t)]$$



- Propagation

$$f_i(\mathbf{r}+\mathbf{e}_i\Delta t, t+\Delta t) = f_i^c(\mathbf{r},t)$$



The LBE with the forcing term

The evolution equation becomes

$$f_i(\mathbf{r}+\mathbf{e}_i\Delta t, t+\Delta t) - f_i(\mathbf{r},t) = -\frac{\Delta t}{\tau}[f_i - f_i^{eq}] + \Delta t F_i$$

- The forcing term F_i depends on the force density $\mathbf{F}$ acting on the fluid
- F_i can be expressed as a power series at the second order in the lattice velocity and is determined by requiring that its moments are consistent with the hydrodynamic equations
- The fluid momentum is redefined as

$$n\mathbf{u}^* = \sum_i f_i \mathbf{e}_i + \frac{1}{2}\mathbf{F}\Delta t,$$

This corresponds to an average between the pre- and post-collisional values

- f_i^{eq} are NOT modified with respect to the standard LBE except for the formal substitution $\mathbf{u} \rightarrow \mathbf{u}^*$

The continuum limit

By using a Chapman-Enskog expansion the continuity equation and the following NS equation are obtained

$$\partial_t(nu^*_\beta) + \partial_\alpha(nu^*_\alpha u^*_\beta) = -\partial_\beta(nc_s^2) + F_\beta +$$

$$+\partial_\alpha[\eta(\partial_\alpha u^*_\beta + \partial_\beta u^*_\alpha)]$$

$c_s = c/\sqrt{3}$ is the sound speed of the model

- In the present model it is $\zeta = \eta$
- The viscosity is

$$\eta = nc_s^2\Delta t(\frac{\tau}{\Delta t} - \frac{1}{2})$$

- To recover the correct NS equation it has to be

$$\mathbf{F} = -\phi\nabla\mu = -\phi\nabla\left[a\phi + b\phi^3 - \kappa\nabla^2\phi\right]$$

where ϕ comes from the solution of the CD equation

How to compute these derivatives?

Numerical calculation of the forcing term

We use finite-difference schemes defined over 9 lattice sites for the first derivative and the Laplacian

$$\partial_{Dx} = \frac{1}{\Delta x} \begin{bmatrix} -M & 0 & M \\ -N & 0 & N \\ -M & 0 & M \end{bmatrix}$$

$$\nabla^2_D = \frac{1}{\Delta x^2} \begin{bmatrix} R & Q & R \\ Q & -4\,(Q+R) & Q \\ R & Q & R \end{bmatrix}$$

with $2N + 4M = 1$ and $Q + 2R = 1$ to guarantee consistency between the continuous and discrete operators

The standard central difference schemes correspond to the choices $N = \frac{1}{2}, M = 0$ and $Q = 1, R = 0$

The free parameters N and Q are chosen to minimize the spurious velocities

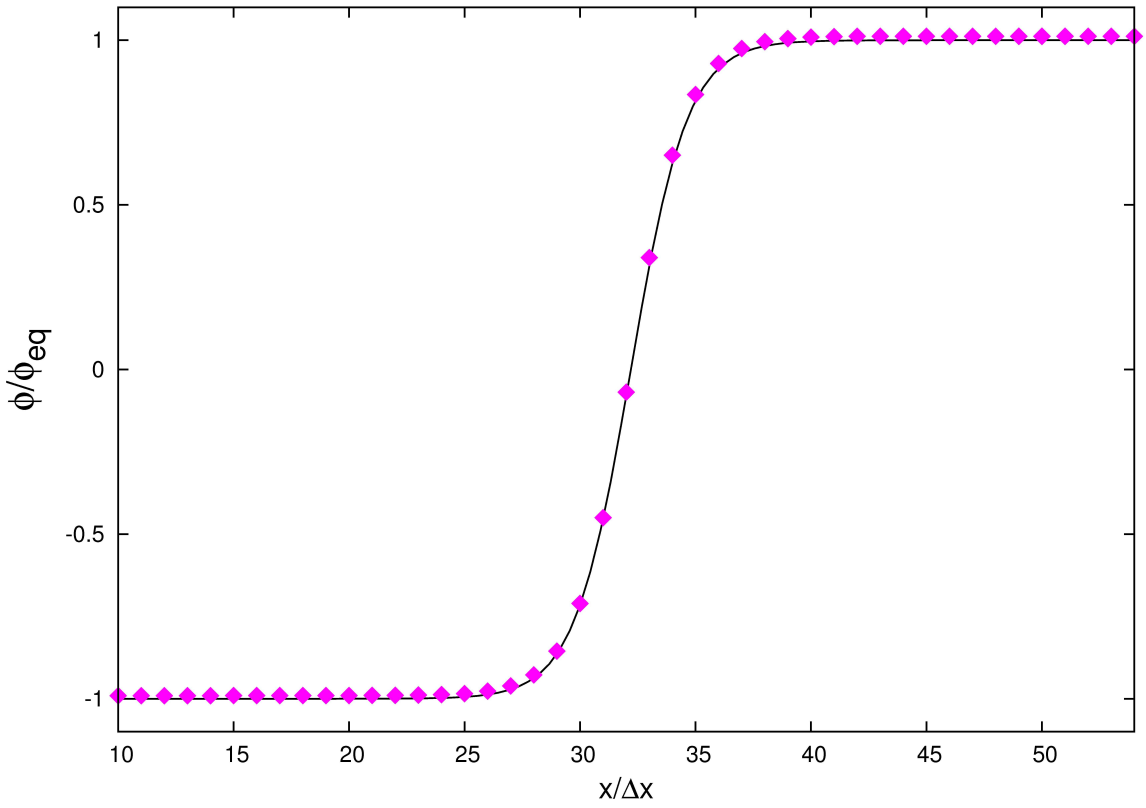
Numerical scheme for the CD equation

- ϕ is defined on the nodes of the LBE lattice
- A standard finite-difference scheme on nearest neighbors for spatial differential operators is adopted
- Time is discretized in steps $\Delta t^{'}$ with $\Delta t = m\Delta t^{'}$ and m integer
- ϕ is updated from time t to $t+\Delta t^{'}$ in two successive partial steps to have a better numerical stability using an explicit first order Euler scheme
  - First we implement the advection term where the velocity $\mathbf{u}^{*}$ comes from the solution of the LBE
  - Then the diffusive part is integrated

Numerical validation

Results were obtained with $\Delta x = \Delta t = \Delta t^{'} = 1$

Relaxation of a planar interface of width $\sim 5\Delta x$ with standard finite differences for the force term in LBE

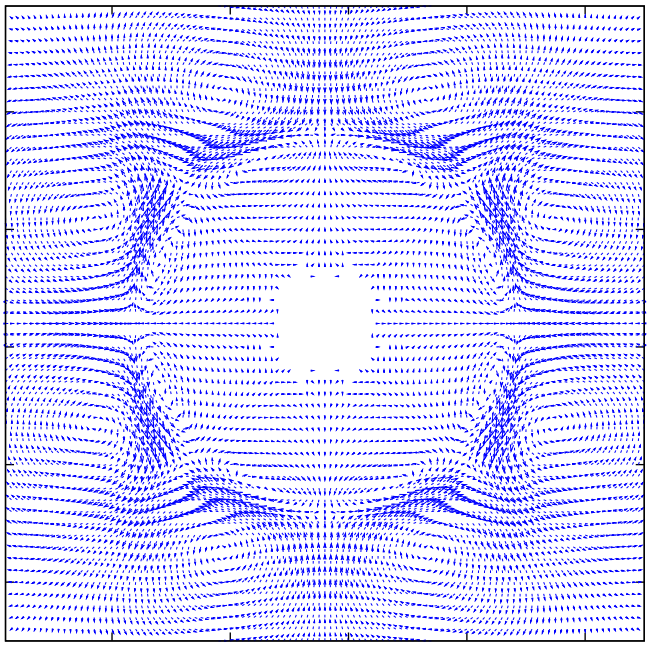


The full line is the analytical solution

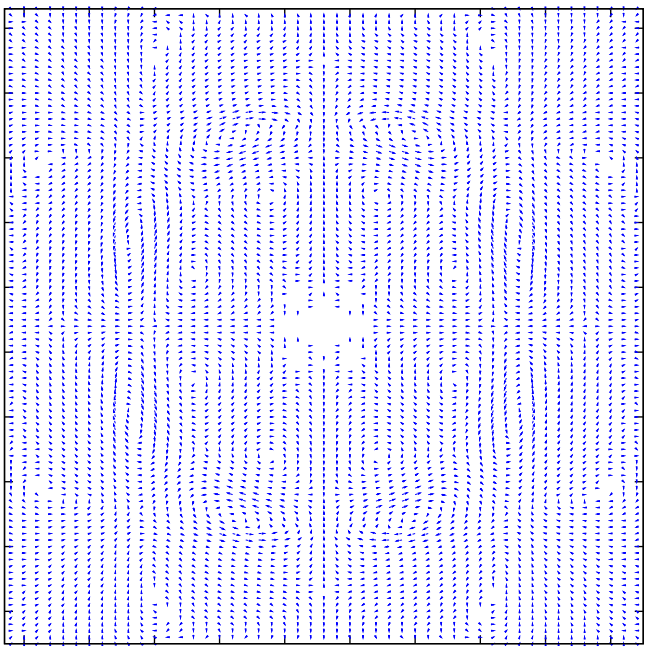
Data points are the simulation results

Equilibration of a droplet on a 128×128 lattice

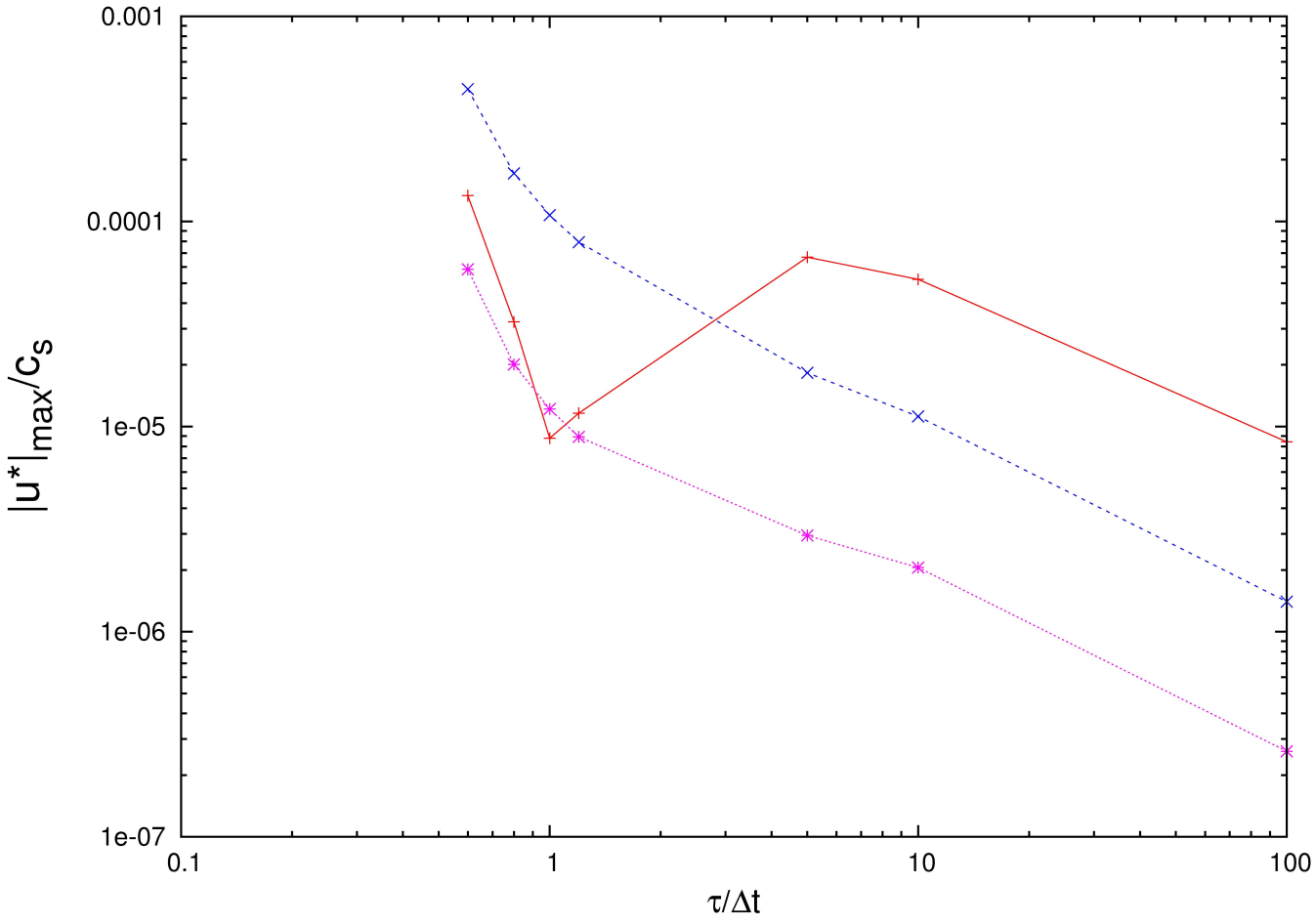
Velocities in the standard case for the force term



Velocities with the optimal choice for the force term



Spurious velocities



Yeomans model

Our model with the standard choice $N = 1/2, Q = 1$

Our model with the optimal choice $N = 0.3, Q = 2.5$

The optimal parameters are valid over the range

$0.6 < \tau/\Delta t < 100$

Conclusions and Perspectives

- The present model takes into account thermodynamics via a forcing term in the LBE
- The correct NS equation is recovered
- Spurious velocities can be reduced using a 9-point stencil for the space derivatives
- The CD equation can be integrated on the same space and time scales of the LBE

- Application to complex fluids
- Extension to thermal binary fluids