Electronic Supplementary Information: Active nematic-isotropic interfaces in channels

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We describe the details of the multi-relaxation-time lattice Boltzmann method used in the simulations and the parameters of the systems illustrated in the videos in the ESI.

1 Description of the videos

The three videos illustrate the results of simulations running up to $t = 500000$ with interval between the frames of $\Delta t = 5000$. The parameters and initial condiitons are described in Sec. 3.1 of the paper.

video1.gif. Interfacial dancing state for homeotropic anchoring (fig. 3C of the paper). Here $\zeta = 0.002$, $\xi = 0.7$.

video2.gif. Interfacial dancing state for planar anchoring (fig. 12C of the paper). Here $\zeta = 0.0025$, $\xi = 0.5$.

video3.gif. Interfacial instability at a closed channel with nematic left boundary and isotropic right boundary (fig. 13 D-G). No slip boundary conditions are applied at the four walls. Here $\zeta = -0.002$, $\xi = 0.5$.

2 The MRT collision operator

As described in the paper, the lattice-Boltzmann equation with the MRT collistion operator reads as follows:

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) - f_i(\mathbf{x},t) = \mathbf{M}^{-1}\mathbf{R}\mathbf{M}[f_i(\mathbf{x},t) - f_i^{eq}(\mathbf{x},t)]\Delta t + \mathscr{S}_i, \tag{1}$$

where the transformation matrix $\mathbf{M}$ transforms the populations space into the moments space, the relaxation matrix $\mathbf{R}$ includes the relaxation rates of the individual moments and $\mathscr{S}_i$ is the souce term. In the simplest form (first order accurate), the source term is $\mathscr{S}_i = 3w_i\mathbf{F}\cdot\mathbf{c}_i$. In our simulations, we projected the Guo's forcing term in the moments space using the matrix $\mathbf{M}$, similarly as done for the populations. This procedure is described in Chapter 10 of Ref.[1]. For an implementation of the MRT in the D3Q19 lattice in C++, we recommend Palabos[2]. The matrices and vectors are given below.

The velocity vetors for the D3Q19 are given by:

$$c_x = [0,-1,0,0,-1,-1,-1,-1,0,0,1,0,0,1,1,1,1,0,0]$$

$$c_y = [0,0,-1,0,-1,1,0,0,-1,-1,0,1,0,1,-1,0,0,1,1]$$

$$c_z = [0,0,0,-1,0,0,-1,1,-1,1,0,0,1,0,0,1,-1,1,-1].$$

The discrete weight associated with each vector depends on its length: $w(0) = 1/3$, $w(1) = 1/18$ and $w(2) = 1/36$. The transformation

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matrix is:

$$
\mathbf{M} = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-30 & -11 & -11 & -11 & 8 & 8 & 8 & 8 & 8 & 8 & -11 & -11 & -11 & 8 & 8 & 8 & 8 & 8 & 8 \\
12 & -4 & -4 & -4 & 1 & 1 & 1 & 1 & 1 & 1 & -4 & -4 & -4 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & -1 & 0 & 0 & -1 & -1 & -1 & -1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\
0 & 4 & 0 & 0 & -1 & -1 & -1 & -1 & 0 & 0 & -4 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 & -1 & 1 & 0 & 0 & -1 & -1 & 0 & 1 & 0 & 1 & -1 & 0 & 0 & 1 & 1 \\
0 & 0 & 4 & 0 & -1 & 1 & 0 & 0 & -1 & -1 & 0 & -4 & 0 & 1 & -1 & 0 & 0 & 1 & 1 \\
0 & 0 & 0 & -1 & 0 & 0 & -1 & 1 & -1 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & -1 & 1 & -1 \\
0 & 0 & 0 & 4 & 0 & 0 & -1 & 1 & -1 & 1 & 0 & 0 & -4 & 0 & 0 & 1 & -1 & 1 & -1 \\
0 & 2 & -1 & -1 & 1 & 1 & 1 & 1 & -2 & -2 & 2 & -1 & -1 & 1 & 1 & 1 & 1 & -2 & -2 \\
0 & -4 & 2 & 2 & 1 & 1 & 1 & 1 & -2 & -2 & -4 & 2 & 2 & 1 & 1 & 1 & 1 & -2 & -2 \\
0 & 0 & 1 & -1 & 1 & 1 & -1 & -1 & 0 & 0 & 0 & 1 & -1 & 1 & 1 & -1 & -1 & 0 & 0 \\
0 & 0 & -2 & 2 & 1 & 1 & -1 & -1 & 0 & 0 & 0 & -2 & 2 & 1 & 1 & -1 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & -1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1
\end{bmatrix} \tag{2}
$$

The equilibrium moments are:

$$
\mathbf{m^{eq}} = \begin{bmatrix}
\rho \\
\rho(-11 + 19u_x^2 + 19u_y^2 + 19u_z^2) \\
-\frac{1}{2}\rho(-6 + 11u_x^2 + 11u_y^2 + 11u_z^2) \\
\rho u_x \\
-\frac{2}{3}\rho u_x \\
\rho u_y \\
-\frac{2}{3}\rho u_y \\
\rho u_z \\
-\frac{2}{3}\rho u_z \\
\rho(2u_x^2 - u_y^2 - u_z^2) \\
\frac{1}{2}\rho(-2u_x^2 + u_y^2 + u_z^2) \\
\rho(u_y^2 - u_z^2) \\
\frac{1}{2}\rho(-u_y^2 + u_z^2) \\
\rho u_x u_y \\
\rho u_y u_z \\
\rho u_x u_z \\
0 \\
0 \\
0
\end{bmatrix} \tag{3}
$$

And the force term in the moment space is $\mathbf{MF}' = (\mathbf{I}-\mathbf{R}/2)\,\mathbf{S}$, where:

$$\mathbf{S} = \begin{bmatrix} 0 \\ 38(F_x u_x + F_y u_y + F_z u_z) \\ -11(F_x u_x + F_y u_y + F_z u_z) \\ F_x \\ -\frac{2}{3}F_x \\ F_y \\ -\frac{2}{3}F_y \\ F_z \\ -\frac{2}{3}F_z \\ 2(2F_x u_x - F_y u_y - F_z u_z) \\ (-2F_x u_x + F_y u_y + F_z u_z) \\ 2(F_y u_y - F_z u_z) \\ -F_y u_y + F_z u_z \\ F_y u_x + F_x u_y \\ F_z u_y + F_y u_z \\ F_z u_x + F_x u_z \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{4}$$

We use the relaxation rates of Ref.[3], which have been shown to reduce significantly the spurious velocities in a multiphase pseudopotential model for simple fluids.

$$\mathbf{R} = \mathrm{diag}(\omega_0, \omega_1, \ldots, \omega_{18}) \tag{5}$$

where: $\omega_0 = \omega_3 = \omega_5 = \omega_7 = \omega_{10} = \omega_{12} = \omega_{16} = \omega_{17} = \omega_{18} = 1$ and $\omega_1 = \omega_2 = \omega_4 = \omega_6 = \omega_8 = 1.1$. The parameters $\omega_9 = \omega_{13} = \omega_{14} = \omega_{15}$ are related to the kinematic viscosity: $\nu = c_s^2\left(\frac{1}{\omega_9} - \frac{1}{2}\right)$, while the ω_1 is related to the bulk viscosity: $\eta_B = \rho c_s^2\left(\frac{1}{\omega_1} - \frac{1}{2}\right) - \frac{\nu\rho}{3}$.

Notes and references

1 T. Krüger, H. Kusumaatmaja, A. Kuzmin, O. Shardt, G. Silva and E. M. Viggen, *The Lattice Boltzmann Method - Principles and Practice*, Springer International Publishing, 2016.

2 *Palabos*, `http://www.palabos.org`.

3 S. Ammar, G. Pernaudat and J.-Y. Trépanier, *Journal of Computational Physics*, 2017, **343**, 73 – 91.