Two-dimensional hybrid lattice Boltzmann code for active nematodynamics

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This document is a part of a programming package to simulate two-dimensional active nematics. The numerical package aims to give an introduction into the hybrid lattice Boltzmann method and numerical modelling of active nematics. When using the code, please cite directly this upload or Ref. [1].

Numerical package

The code is writen in C programming language. It uses a D2Q19 lattice Boltzmann model combined with a finite difference approach for the Q-tensor. Periodic boundary conditions are used. The numerical code simulates a simplified continuus dynamics of the Q-tensor for an incompressible active nematic [2–4]:

$$\rho\frac{\mathrm{d}v_i}{\mathrm{d}t} = \eta\nabla^2 v_i - \partial_i p + \partial_j\sigma_{ij}, \tag{1}$$

$$\frac{\mathrm{d}Q_{ij}}{\mathrm{d}t} = \lambda u_{ij} + Q_{ik}\omega_{kj} - \omega_{ik}Q_{kj} + \frac{1}{\gamma}H_{ij}, \tag{2}$$

where ρ is density, $\boldsymbol{v}$ velocity, t time, η viscosity, p pressure, σ_{ij} the stress tensor, Q_{ij} the nematic tensor order parameter, λ the alignment parameter, $u_{ij} = (\partial_i v_j + \partial_j v_i)/2$, $\omega_{ij} = (\partial_i v_j - \partial_j v_i)/2$, γ the rotational viscosity, and $H_{ij} = -\frac{\delta f}{\delta Q_{ij}}$ the molecular field. The stress tensor equals

$$\sigma_{ij} = -\lambda H_{ij} + Q_{ik}H_{kj} - H_{ik}Q_{kj} + \alpha Q_{ij}, \tag{3}$$

where α is the activity. The free energy density equals

$$f = \frac{L}{2}(\partial_k Q_{ij})^2 + CQ_{ij}Q_{ji}(Q_{ij}Q_{ji} - 1), \tag{4}$$

where L is the elastic constant and C the phase parameter.

The parameter values of the simulated equations can be tuned in the file *parameters.c*. Given the values of the variables in the files, the above parameters can be expressed in units of spatial resolution Δx, L and γ:

$$\begin{aligned}&\Delta t = \mathrm{DT}\frac{\Delta x^2\gamma}{L}\,,\lambda = \mathrm{LAMBDA}\,,\rho = \mathrm{DENSITYINIT}\cdot\mathrm{DT}^2\frac{\gamma^2}{L}\,,\\ &\eta = \mathrm{DENSITYINIT}\cdot\mathrm{DT}\frac{1}{3}\left(\frac{\mathrm{TAUF}}{\mathrm{DT}} - \frac{1}{2}\right)\gamma\,,\alpha = \mathrm{ALPHA}\frac{L}{\Delta x^2}\,,C = \mathrm{C}\frac{L}{\Delta x^2}\end{aligned} \tag{5}$$

The velocity field is given in units of $\Delta x/\Delta t$.

Exercises

Here, we give a few potential exercises that lead the user of the programming package to get accustomed to the numerical code, modelling approach, and some common properties two-dimensional active nematodynamics.

1. Run the code at some selected values of the parameters in the file "parameters.c". The prescribed values should work well on a laptop, but if you wish, you can change the system size and other parameters as well.

   (a) For the prescribed values, the system reaches a dynamical steady state in about 30000 time steps. Wait until your system reaches a dynamical steady state and plot the velocity, director, and the scalar degree of order fields. Describe what you see.

(b) Define and compute the dimensionless numbers, such as Ericksen number and Reynolds number for some typical length scale in the steady state regime.

2. Find where in the code the initial conditions for the Q-tensor and the velocity field field are prescribed. Set the initial velocity to zero.

   (a) Change the director initial condition to a homogeneous field with some small perturbation in the middle. Follow how the director and the velocity structure evolves at medium activity (ALPHA ≈ 0.25) and at large activity (ALPHA ≈ 1). Describe what you see.

   (b*) Change the Q-tensor initial condition to a $\pm 1/2$ defect pair at some distance. Hint: planar director field with defects can be initialized from a linear superposition of the director angles θ_1 and θ_2, where θ_1 corresponds to director profile of a defect at location $\boldsymbol{r}_1$ and θ_2 to a defect at $\boldsymbol{r}_2$. Plot the annihilation dynamics of a defect pair at a few different activities.

3. Generate the dynamical steady state known also as active turbulence at various activities.

   (a) How does the number of defects scale with activity? Hint: defect positions are easily recognizable as minima in the scalar degree of order field. You can estimate the number of defects from the number of mesh points with the degree of order below some threshold value. You might want to increase the time step and the simulation box to get a better statistics.

   (b**) Plot the power spectrum of the kinetic energy at some high activity [2, 5]. Do you observe a characteristic scaling at large wavelengths? Compare to Ref. [2]. You might have to use a larger simulation box to get better results.

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