Supplementary Information

LM14989 - "Defect-mediated morphologies in growing cell colonies", by
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Lattice-Boltzmann simulation of two-phase flow of the mixture of active nematics and an isotropic fluid

The equations (1-3) of the manuscript are solved using hybrid Lattice-Boltzmann method. To this end, equations (1,2) are solved by a finite difference scheme using a five-point stencil to discretise the derivatives on a square grid. These are coupled to Navier-Stokes equations, that are solved using Lattice-Boltzmann (LB) method with the Bhatnagar-Gross-Krook (BGK) approximation and a single relaxation time for the collision operator [1–8]. The time integration is performed using PECE predictor-corrector method. The discrete space and time steps are chosen as unity for the LB method. The algorithm is implemented using C++ programming language.

All simulations were performed on a 800×800 square grid with periodic boundary conditions on the domain boundaries. All simulations were started with an initial circular colony of the radius $R = 10$ (in LB units) with $\phi = 1$ and random orientation field, while at the beginning of the simulation the velocity field was set to zero everywhere in the domain. The random orientations were created using drand48() function of the C++ library. In all simulations, the parameters were set to $\rho = 1$, $\Gamma_Q = 0.025$, Γ_φ=0.1, $K_\varphi = 0.05$, $K = 0.01$, $\alpha = 0.0001$, $\lambda = 0.3$, $q_n = 1$, $A = 0.8$, $A_\varphi = 0.6$, $\eta = 2/3$, $t_0 = 1000$, and $r_0 = 5$, in lattice units and the friction coefficient was varied in Figs. 2, 3, 4b, 5. The corresponding friction coefficients are listed in the legends of figures in the main text. We have chosen parameters in a range that has previously been successful in reproducing the velocity correlations observed in experiments on microtuble bundles [9, 10] and in reproducing the flow fields of dividing MDCK cells [11].

For each of the data presented in Fig. 3, Fig. 4b, and Fig. 5 of the main text, twenty separate simulations with different random orientations were performed and the resulting mean values were presented in the figures. In Fig. 3a the error bars were calculated based on the standard deviations of data at each point from its corresponding mean value of twenty simulations for that specific point.

All simulations were run for up to 2×10^7 simulation time steps. In Fig. 2, the snapshots from left to right correspond to simulation times of $t = 0$, 4×10^5, and 7×10^6. The constant values reported in Fig. 3b, and Fig. 3c were calculated after the statistical steady-states for the IQ and N_d were established at the time 1.8×10^7. In Fig. 4a,4c, the snapshots were taken at the simulation time of $t = 5 \times 10^5$ for the case of $f_0 = 0.02$. The distributions reported in Fig. 5 and the cross correlations reported in Fig. 4b, are averaged over the time period of $[2 \times 10^4 - 2 \times 10^7]$.

References

[1] P. G. de Gennes and J. Prost. The Physics of Liquid Crystals. Oxford University Press, 1995.

[2] A. N. Beris and B. J. Edwards. Thermodynamics of Flowing Systems. Oxford University Press, 1994.

[3] C. Denniston, D. Marenduzzo, E. Orlandini, and J. M. Yeomans. Lattice Boltzmann algorithm for three dimensional liquid crystal hydrodynamics. Phil. Trans. R. Soc. A, 362(1821):1745–1754, 2004.

[4] D. Marenduzzo, E. Orlandini, M. E. Cates, and J. M. Yeomans. Steady-state hydrodynamic instabilities of active liquid crystals: Hybrid lattice Boltzmann simulations. Phys. Rev. E, 76:031921, 2007.

[5] S. M. Fielding, D. Marenduzzo, and M. E. Cates. Nonlinear dynamics and rheology of active fluids: Simulations in two dimensions. Phys. Rev. E, 83:041910, 2011.

[6] Sumesh P Thampi, Ramin Golestanian, and Julia M Yeomans. Vorticity, defects and correlations in active turbulence. Phil. Trans. R. Soc. A, 372(2029):20130366, 2014.

[7] L. Giomi, L. Mahadevan, B. Chakraborty, and M. F. Hagan. Excitable patterns in active nematics. Phys. Rev. Lett., 106:218101, 2011.

[8] J. W. Cahn and J. E. Hilliard. Free energy of a nonuniform system. i. interfacial free energy. J. Chem. Phys., 28(2):258–267, 1958.

[9] T. Sanchez, D. T. N. Chen, S. J. DeCamp, M. Heymann, and Z. Dogic. Spontaneous motion in hierarchically assembled active matter. Nature, 491:431–434, 2012.

[10] S. P. Thampi, R. Golestanian, and J. M. Yeomans. Velocity correlations in an active nematic. Phys. Rev. Lett., 111:118101, 2013.

[11] A. Doostmohammadi, S. P. Thampi, T. B. Saw, C. T. Lim, B. Ladoux, and J. M. Yeomans. Celebrating Soft Matter's 10th Anniversary: Cell division: a source of active stress in cellular monolayers. Soft Matter, 11:7328–7336, 2015.