Supplementary Information

for manuscript *Surface anchoring controls orientation of a microswimmer in nematic liquid crystal*, by H. Chi, M. Potomkin, L. Zhang, L. Berlyand and I. S. Aranson

Note that all equation numbers below refer to equations in the main text, unless the number has prefix "SI-"

Supplementary Note 1: Expressions for S, $\boldsymbol{\sigma}_a$, and $\boldsymbol{\sigma}_s$ in Beris-Edwards model

The term $\mathbf{S}(\nabla\mathbf{v},\mathbf{Q})$ from (6) is defined by

$$\mathbf{S}(\nabla\mathbf{v},\mathbf{Q}) = (\xi\mathbf{A}+\boldsymbol{\Omega})(\mathbf{Q}+\frac{1}{d}\mathbf{I}) + (\mathbf{Q}+\frac{1}{d}\mathbf{I})(\xi\mathbf{A}-\boldsymbol{\Omega}) \\ -2\xi(\mathbf{Q}+\frac{1}{d}\mathbf{I})\mathrm{tr}(\mathbf{Q}\nabla\mathbf{v}),$$

where $\mathbf{A}=(\nabla\mathbf{v}+\nabla\mathbf{v}^{\mathrm{T}})/2$ and $\boldsymbol{\Omega}=(\nabla\mathbf{v}-\nabla\mathbf{v}^{\mathrm{T}})/2$ are the symmetric and anti-symmetric part of $\nabla\mathbf{v}$, respectively; parameter $\xi\in[0,1]$ depends on shape properties of LC molecules or, in other words, ξ measures the ratio between the tumbling and the aligning effects that a shear flow exerts on the LC director field.

The term $\boldsymbol{\sigma}_{LC}$ from (7) is defined by $\boldsymbol{\sigma}_{LC}=\boldsymbol{\sigma}_a+\boldsymbol{\sigma}_s$, where $\boldsymbol{\sigma}_a$ and $\boldsymbol{\sigma}_s$ are anti-symmetric and symmetric parts of $\boldsymbol{\sigma}_{LC}$, respectively, given by

$$\boldsymbol{\sigma}_a = \mathbf{QH}-\mathbf{HQ},$$
$$\boldsymbol{\sigma}_s = -\xi\mathbf{H}(\mathbf{Q}+\frac{1}{d}\mathbf{I}) - \xi(\mathbf{Q}+\frac{1}{d}\mathbf{I})\mathbf{H} + 2\xi(\mathbf{Q}+\frac{1}{d}\mathbf{I})\,\mathrm{tr}(\mathbf{QH}) - K\nabla\mathbf{Q}\odot\nabla\mathbf{Q}.$$

Here, $(\nabla\mathbf{Q}\odot\nabla\mathbf{Q})_{ij}=\sum_{k,l}Q_{kl,i}Q_{kl,j}$.

Supplementary Note 2: Torque balance for microswimmer in LC

In this supplementary subsection we show the derivation of the torque balance (13)-(14) for the microswimmer immersed in LC. This is done by using the energy principle. Namely, in the case of a passive microswimmer, occupying region $\mathcal{B}(t)$ at time t, the total energy of the system consisting of microswimmer and LC dissipates according to

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\mathcal{K}+\mathcal{E}_{\mathbf{Q}}\right]+\mathcal{D}=0. \tag{SI-1}$$

Here $\mathcal{K}=m_{\mathrm{sw}}(\dot{\mathbf{x}}_c)^2/2+\mathrm{I}_{\mathrm{sw}}(\dot{\alpha})^2/2+\rho_{\mathrm{LC}}/2\int|\mathbf{v}|^2\,\mathrm{d}\mathbf{x}$ is the total kinetic energy of the system (m_{sw}, I_{sw}, and ρ_{LC} are microswimmer's mass, microswimmer's moment of inertia, and LC density, respectively), $\mathcal{E}_{\mathbf{Q}}$ is the total free energy defined by (11) and $\mathcal{D}$ is the dissipation of energy of the system and is given by (see, e.g., [1, 2]):

$$\mathcal{D}=\int \eta|\mathbf{A}|^2+\Gamma|\mathbf{H}|^2\,\mathrm{d}\mathbf{x},\ \text{where } \mathbf{A}=(\nabla\mathbf{v}+\nabla\mathbf{v}^{\mathrm{T}})/2.$$

On the other hand, if one computes the time derivative $\frac{\mathrm{d}}{\mathrm{d}t}\left[\mathcal{K}+\mathcal{E}_{\mathbf{Q}}\right]$, uses (6), (7), (8), (1) with $v_0=0$, and (3), as well as Reynolds transport formulas to treat integrals over time dependent domains, and integration by parts, then one obtains the following:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\mathcal{K}+\mathcal{E}_{\mathbf{Q}}\right]+\mathcal{D}=\dot{\mathbf{x}}_c\cdot\left[m_{\mathrm{sw}}\,\ddot{\mathbf{x}}_c+\int\limits_{\mathcal{S}(t)}\mathbf{F}_\nu\,\mathrm{d}S_{\mathbf{x}}\right]$$
$$+\,\dot{\alpha}\left[\mathrm{I}_{\mathrm{sw}}\ddot{\alpha}+\mathbf{e}_z\cdot\int\limits_{\mathcal{S}(t)}\left[(\mathbf{x}-\mathbf{x}_c(t))\times\mathbf{F}_\nu+\boldsymbol{\ell}\right]\mathrm{d}S_{\mathbf{x}}\right], \tag{SI-2}$$

where $\boldsymbol{\ell}$ is defined by (14). By substituting (12), (SI-1) into (SI-2) we obtain torque balance (13). Note that since we study microswimmers, inertia terms are neglected, that is, $m_{\mathrm{sw}}=\mathrm{I}_{\mathrm{sw}}=0$ in (12) and (13).

We also describe an alternative approach to find the expression for $\boldsymbol{\ell}$. Consider a continuum media in the presence of couple stresses described by tensor $\boldsymbol{\mu}$, which means that couple stresses exert a torque $\boldsymbol{\ell}=\boldsymbol{\mu}\boldsymbol{\nu}$ on the surface element with normal vector $\boldsymbol{\nu}$. Take an arbitrary domain V, enclosed by surface S. Without loss of generality, assume that 0 lies inside V. Torque balance around point 0 takes the form:

$$0=\int\limits_S \epsilon_{ijk}x_j\sigma_{kl}\nu_l+\mu_{il}\nu_l\,\mathrm{d}S_{\mathbf{x}}+\int\limits_V\left(\epsilon_{ijk}x_jF_k\right)\mathrm{d}\mathbf{x}. \tag{SI-3}$$

Here ϵ_{ijk} is the Levi-Civita symbol ($(\boldsymbol{a}\times\boldsymbol{b})\cdot\boldsymbol{e}_i=\epsilon_{ijk}a_jb_k$), $\boldsymbol{F}$ represents body forces. From the force balance it follows that

$$\sigma_{km,m}+F_k=0. \tag{SI-4}$$

Integration by parts in (SI-3) yields:

$$0=\int\limits_V\left(\epsilon_{ijk}\sigma_{jk}+\mu_{il,l}\right)\mathrm{d}\mathbf{x}+\int\limits_V\epsilon_{ijk}x_j\left(\sigma_{km,m}+F_k\right)\mathrm{d}\mathbf{x}.$$

Force balance equation (SI-4) implies that the second integral above vanishes, and due to arbitrariness of domain V we get an equation for couple-stress:

$$\mu_{il,l}=-\epsilon_{ijk}\sigma_{jk}. \tag{SI-5}$$

In the framework of the Beris-Edwards model, one can find such tensor $\boldsymbol{\mu}$ that (SI-5) holds for $\boldsymbol{\sigma}=\boldsymbol{\sigma}_{LC}$. Specifically,

$$\mu_{il}=-2K\epsilon_{ijk}Q_{jm}Q_{mk,l}.$$

Finally, by using $\boldsymbol{\ell}=\boldsymbol{\mu}\boldsymbol{\nu}$ and (3) one can verify formula (14).

Supplementary Note 3: Effective orientation dynamics in the limit Er $\to 0$

Here, we provide arguments how to justify equation (5) in the limit Er $\to 0$. We make an approximating assumption that we can represent the torque balance exerted by LC on the microswimmer as

$$0 = \mathrm{T}_{\mathrm{visc}} + \mathrm{T}_{\mathrm{active}} + \mathrm{T}_{\mathrm{stab}} \tag{SI-6}$$

That is, the net torque consists of the viscous drag torque, active torque reorienting the pusher or the puller as if the microswimmer is symmetric (spherical), and the stabilizing torque which acts on the microswimmer since it has a major axis (elongated) whereas the surrounding environment has a preferred direction. Here equation (SI-6) is scalar since all rotations occur around z-axis. Following [3], we have:

$$\mathrm{T}_{\mathrm{visc}} = -\kappa_1 \eta L^3 \dot{\alpha} \text{ and } \mathrm{T}_{\mathrm{active}} = \kappa_2 v_0 \beta L^2 \eta \sin(2\alpha), \tag{SI-7}$$

where κ_1 and κ_2 are coefficients accounting that effective viscosities, $\hat{\eta}$ and $\hat{\eta}_\Omega$, computed in [3] are different from η.

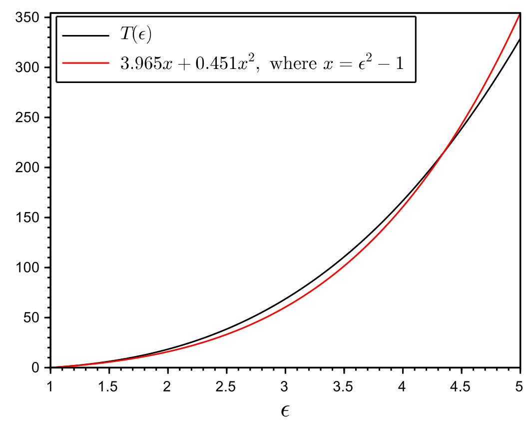
The stabilizing torque is given by

$$\mathrm{T}_{\mathrm{stab}} = \boldsymbol{\ell} \cdot \boldsymbol{e}_z = 2\frac{K\hat{W}}{L} \int\limits_{\partial\mathcal{E}} R\left(\frac{\pi}{2}\right) Q_{\mathrm{anchor}} : Q \, \mathrm{d}S_x.$$

Here $\hat{W} = WL/K$. In the limit Er $\to 0$, assume that $Q = \boldsymbol{e}_1 \otimes \boldsymbol{e}_1 - \mathrm{I}/2$. Then

$$\mathrm{T}_{\mathrm{stab}} = -2\frac{K\hat{W}}{L} \int\limits_{\partial\mathcal{E}} \tau_1 \tau_2 \, \mathrm{d}S_x,$$

where τ_1 and τ_2 are components of the tangent vector $\boldsymbol{\tau}$. By straightforward calculations one gets



Supplementary Figure 1: Dependence of parameter T on aspect ratio ϵ

$$\mathrm{T}_{\mathrm{stab}} = -2K\hat{W}LT(\epsilon)\sin 2\alpha,$$

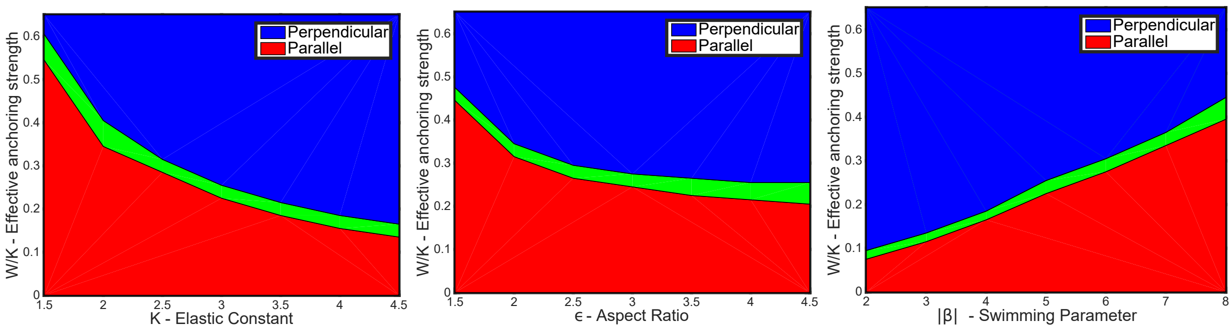
where $T(\epsilon) = 2\int\limits_0^\pi \left((\epsilon^2-1)\sin^2\theta + 2\sin^2\theta - 1\right)\sqrt{(\epsilon^2-1)\sin^2\theta + 1}\,\mathrm{d}\theta$ is a monotonically increasing function of ϵ, see Supplementary Figure 1, such that $T(\epsilon = 1) = 0$, that is, in the case of spherical microswimmer the stabilizing torque vanishes.

Combining all expressions for torques we get:

$$\dot{\alpha} = \frac{2T(\epsilon)}{\kappa_1 L \eta}\left(\frac{\kappa_2 v_0 \beta \eta}{T(\epsilon)} - W\right)\sin(2\alpha). \tag{SI-8}$$

This equation becomes (5) with $\gamma = \dfrac{2T(\epsilon)}{\kappa_1 L \eta}$ and $W_c = \dfrac{\kappa_2 v_0 \beta \eta}{T(\epsilon)}$.

Supplementary Note 4: Numerical simulations for pusher with homeotropic surface anchoring



Supplementary Figure 2: **Critical anchoring strength for pusher.** Dependence of the critical anchoring strength *of pusher with homeotropic anchoring* on elastic constant K (a), microswimmer's aspect ratio ϵ (b), and swimming parameter β (c). Blue and red zones correspond to $\alpha(t) \to \pi/2$ and $\alpha(t) \to 0$ as $t \to \infty$, respectively. Green zone stands for those parameters regime for which $\alpha(t)$ varies slowly and does not exhibit clear convergence as $t \to \infty$. Parameters, if not varied (like, e.g., K in (a)), are chosen as follows: $\eta = 5.0, \quad \epsilon = 3.0, \quad L = 1.0, \quad \beta = -5.0, \quad K = 3.0, \quad v_0 = 0.1$.

Supplementary references:

[1] M. Paicu and A. Zarnescu. Global existence and regularity for the full coupled Navier-Stokes and Q-tensor system. *SIAM Journal on Mathematical Analysis*, 43(5):2009–2049, 2011.

[2] M. Paicu and A. Zarnescu. Energy dissipation and regularity for a coupled Navier-Stokes and Q-tensor system. *Archive for Rational Mechanics and Analysis*, 203(1):45–67, 2012.

[3] J. S. Lintuvuori, A. Würger, and K. Stratford. Hydrodynamics defines the stable swimming direction of spherical squirmers in a nematic liquid crystal. *Physical review letters*, 119(6):068001, 2017.