Supporting Information: Viscotaxis of Beating Flagella

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S1. LIST OF PARAMETERS

Parameters	Symbol	Value
Particle number	N	314
Bond length	b	1.0
Flagellum length	L	314.0
Mass	m	1.0
Beat period	τ_0	10^4
Time step	dt/τ_0	5×10^{-8}
Friction anisotropy	$\xi_{\perp 0}/\xi_{\parallel 0}$	1.81
Perpendicular friction coeff.	$\xi_{\perp 0}$	0.1
Parallel friction coeff.	$\xi_{\parallel 0}$	0.05525
Spring constant	kb^2	2×10^5
Bending rigidity	κ_0/L	63.69
Curvature amplitude	A_c	0.02

TABLE S1: Table of key simulation parameters, their descriptions, and respective values used in the model.

S2. VALIDATING FLAGELLAR DYNAMICS: SIMULATIONS VERSUS THEORY

We compare our simulation results with earlier analytical predictions of Gray and Hancock [1]. In the limit of small beat amplitude A_b, the expression for the swimming velocity is [1]

$$v_{flag} = -\frac{1}{2}\left(\frac{\xi_\perp}{\xi_\parallel} - 1\right) A_b^2 \omega q \tag{S1}$$

for the beat pattern $y(x,t) = A_b \sin(qx - \omega t)$ with beat frequency ω and wave number $q = 2\pi/\lambda$. In addition, the curvature and beat amplitudes, A_c and A_b, respectively are related by $A_b = \lambda^2 A_c / 4\pi^2$.

The comparison of the analytical expression for the beat amplitude A_b as a function of curvature amplitude A_c with the simulation results in Fig. S1(a) shows excellent agreement for small curvature amplitudes $A_b/L \lesssim 0.1$. Also, the simulated swimming velocity agrees well with the analytical expression (S1) for smaller amplitudes $A_b/L \lesssim 0.05$, see Fig. S1(b). Deviations for larger beat amplitudes are due to higher-order effects neglected in the analytic model. Thus, our simulation results agree well with established theoretical predictions, validating our model's accuracy in studying flagellum dynamics.

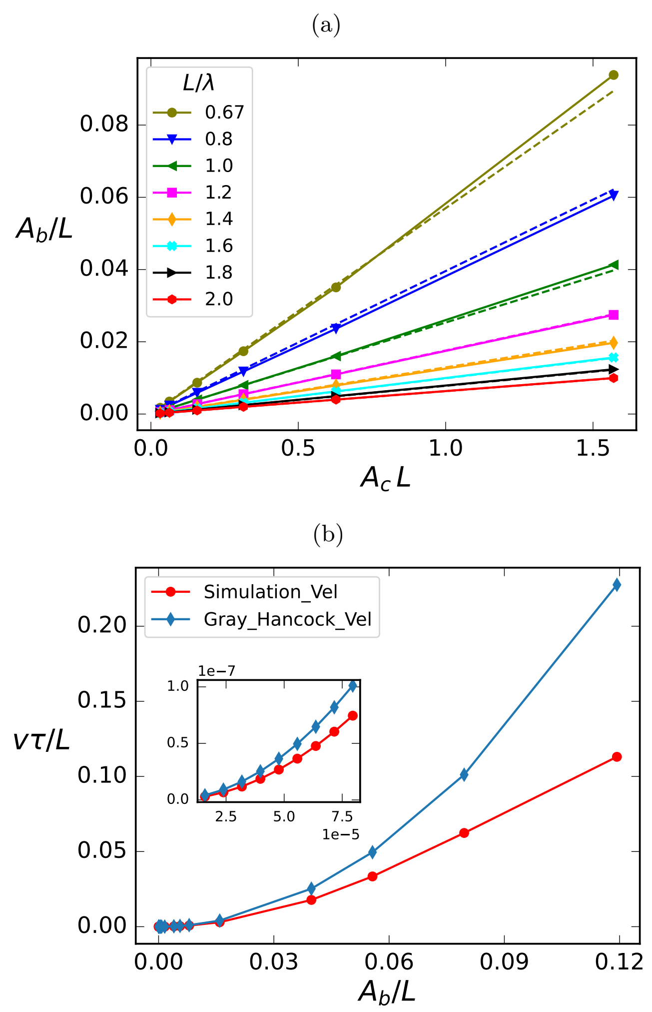

FIG. S1: **Quantitative comparison of simulation results with analytical expressions** (a) Beat amplitude A_b as a function of curvature amplitude A_c, with analytical expression (dashed lines) and simulation results (dotted lines). (b) Propulsion velocity of beating flagellum v_{flag} as a function of beating amplitude A_b.

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S3. ANALYTICAL CALCULATION OF VISCOTACTIC BEHAVIOR

We perform the calculation of the torque induced by a viscosity gradient in a body-fixed reference frame (x', y'), where the x'-axis is along the symmetry axis of the flagellum. We assume a flagellar beat with a simple sinusoidal travelling bending wave,

$$y'(x', t) = A_b \sin(qx' - \omega t) \tag{S2}$$

This implies a mass distribution

$$\rho(x', y', t) = \delta(y' - A_b \sin(qx' - \omega t)) \tag{S3}$$

from which we obtain for a time-averaged beat the projected mass density $\bar{\rho}(y')$ on the y'-axis,

$$\bar{\rho}(y') = \frac{1}{\tau}\int_0^\tau \int_0^L dt\, dx'\, \delta\left(y' - A_b \sin(qx' - \omega t)\right) \tag{S4}$$

The integrations in Eq. (S4) can be performed by using the property of the Dirac's δ function that

$$\delta(g(t)) = \sum_i \frac{1}{|g'(t_{0,i})|}\delta(t - t_{0,i}) \tag{S5}$$

where $t_{0,i}$ are the roots of the function $g(t)$, i.e. $g(t_{0,i}) = 0$. Thus, we have to determine the times t_0 where $y' = A_b \sin(qx' - \omega t_0)$. For y' within the range $[-A_b, A_b]$ and t in $[0, \tau]$ for one wavelength, the above equation has two solutions,

$$\omega t_{0,1} = qx' - \sin^{-1}(y'/A_b) \tag{S6}$$

$$\omega t_{0,2} = qx' - \pi + \sin^{-1}(y'/A_b) \tag{S7}$$

Using the property of the Dirac's δ function given in Eq. (S5), we first integrate over t,

$$\int_0^\tau dt\, \delta(y' - A_b \sin(qx' - \omega t)) = \sum_i \frac{1}{|\omega A_b \cos(qx' - \omega t_{0,i})|} \tag{S8}$$

Hence,

$$\sum_i \frac{1}{|\omega A_b \cos(qx' - \omega t_{0,i})|} = \frac{2}{\omega A_b \sqrt{1 - (y'/A_b)^2}} \tag{S9}$$

The remaining integration over x' finally yields

$$\frac{1}{\tau}\int_0^L dx' \frac{2}{\omega A_b \sqrt{1 - (y'/A_b)^2}} = \frac{L}{\pi\sqrt{A_b^2 - y'^2}} \tag{S10}$$

so that

$$\bar{\rho}(y') = \frac{L}{\pi\sqrt{A_b^2 - y'^2}}. \tag{S11}$$

As a consistency check, we verify that the total mass of the flagellum is

$$\int \bar{\rho}(y')\, dy' = \int_{-A_b}^{A_b} dy' \frac{L}{\pi\sqrt{A_b^2 - y'^2}} = L\,. \tag{S12}$$

The rotational torque T_A required for reorientation of a flagellum then is

$$\begin{aligned}
T_A &= \int_{-A_b}^{A_b} dy'\, y' \bar{\rho}(y')\, v\xi_\parallel \frac{\alpha}{L}\cos(\theta)\, y' \\
&= \frac{\xi_\parallel v\alpha\cos(\theta)}{\pi}\int_{-A_b}^{A_b} dy'\, y'^2 \frac{1}{\sqrt{A_b^2 - y'^2}} \\
&= \frac{\xi_\parallel v\alpha\cos(\theta)}{\pi}\left(\frac{A_b^2}{2}\sin^{-1}(\frac{y'}{A_b}) - \frac{y'}{2}\sqrt{A_b^2 - y'^2}\right)\Bigg|_{-A_b}^{A_b} \\
&= \frac{1}{2} v\alpha\xi_\parallel A_b^2 \cos(\theta)\,,
\end{aligned} \tag{S13}$$

where in the body-fixed reference frame, the gradient direction appears with an angle θ relative to the x'-axis.

The active torque T_A is balanced by the torque T_R due to frictional drag, which for a stiff rod (approximation of very small beat amplitude A_b) around its midpoint is

$$T_R = \Omega\xi_R \simeq \Omega\xi_\perp L^3/12\,. \tag{S14}$$

The resulting angular velocity Ω is then

$$\Omega = 6v\frac{\xi_\parallel}{\xi_\perp}\left(\frac{A_b}{L}\right)^2 \mathbf{P}\times\nabla\left(\frac{\eta}{\eta_0}\right)\,. \tag{S15}$$

Furthermore, Eq. (S15) can be simply re-written as $\Omega(\theta, \alpha) = \Omega_1\alpha\cos(\theta)$, where Ω_1 is the key viscotactic response coefficient. For $\theta \approx 0$, this becomes $\Omega(\alpha) = \Omega_1\alpha$, in good agreement with the simulation results, see Fig. S2(a,b).

To validate our analytical result for Ω, we compared Eq. (S15) with the simulation data in Fig. S3. Both scale with the same power of beat amplitude, $\Omega_1\tau \sim (A_b/L)^4$, as velocity depends quadratically on A_b.

S4. ANALYTICAL CALCULATION OF SWIMMING TRAJECTORY FOR TROCHOID-LIKE MOTION

The orientational motion of an asymmetric flagellum is obtained from the contribution of average spontaneous curvature C_0 and viscosity gradients $\nabla\left(\frac{\eta}{\eta_0}\right)$. As derived in the main text, this motion is described by

$$\dot{\theta} = \Omega_0 + \Omega_1\alpha\cos(\theta) \tag{S16}$$

From the indefinite integral of Eq. (S16) with initial condition $\theta_{init} = 0$ at $t = 0$, we derived the explicit dependence $t(\theta)$ as

$$t(\theta) = \frac{2\tan^{-1}\left(\frac{\sqrt{a-b}}{\sqrt{a+b}}\tan(\frac{\theta}{2})\right) + 2\pi\lfloor\frac{\theta}{2\pi} + \frac{1}{2}\rfloor}{\sqrt{a^2 - b^2}} \tag{S17}$$

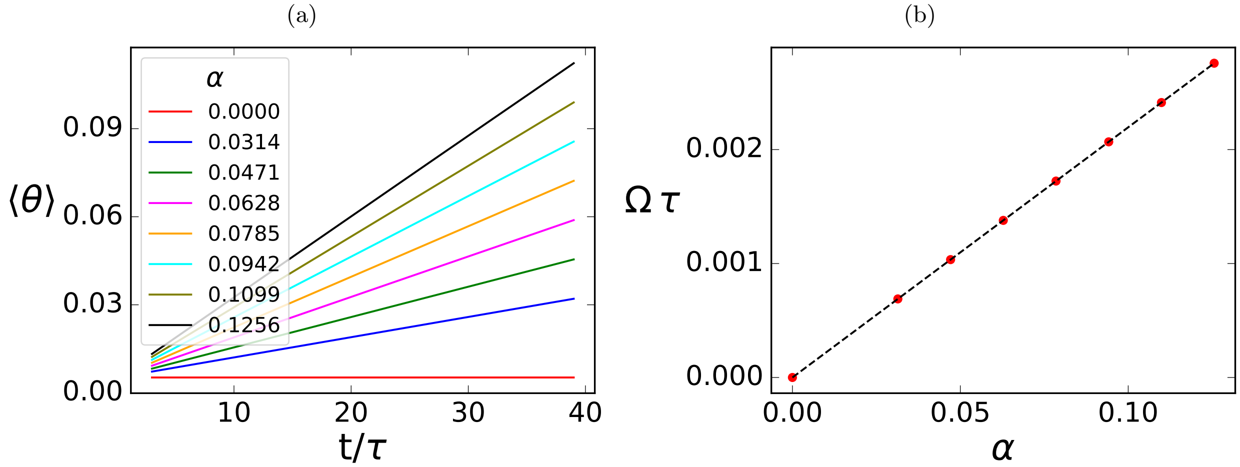

FIG. S2: **Quantifying visotactic behavior.** (a) Averaged orientation of flagellum per beat $\langle\theta\rangle$ (in radians) for different viscosity gradients α as a function of time. (b) Effect of different viscosity gradients on rotational velocity Ω. Data points are obtained from linear fits in (a). The dashed line is linear fit to $\Omega(\alpha) = \Omega_1\alpha$, yielding Ω_1. In (a-b), the initial orientation is chosen to be $\theta \approx 0$. The single fit parameter $\Omega_1\tau = 0.02196$ is the viscotactic response coefficient.

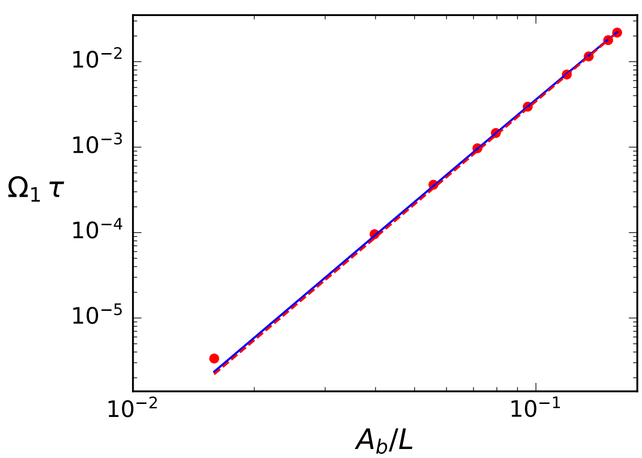

FIG. S3: **Rotational velocity dependence on beat amplitude.** Rotational velocity Ω_1 of the flagellum as a function of beating amplitude for $\alpha = 0.4$. A fit (dashed red lined) of the simulation data (red dot symbols) to the functional dependence $\Omega_1\tau \sim (A_b/L)^4$ (see text) and the analytical predictions (blue solid line) of Eq. (S15) are shown to agree very well.

where, $a = \Omega_0$, $b = \Omega_1\alpha$ and $\lfloor ... \rfloor$ is the floor function. The resulting trochoid-like trajectory is shown in Fig. 10(b) of the main text.

From Eq. (S17), we can easily obtain the time period ΔT of a full cycle by taking the difference of time for θ = 0 and $\theta = 2\pi$, which implies

$$\Delta T = \frac{2\pi}{\sqrt{(\Omega_0)^2 - (\Omega_1\alpha)^2)}} \tag{S18}$$

S5. PROJECTED LENGTH OF FLAGELLUM AS A FUNCTION OF BEATING AMPLITUDE

In order to investigate to which extent the projected length for flagellum L_{eff} (end-to-end distance) is geometrically affected by the beat amplitude A_b, we derive an expression for L_{eff} for small beat amplitudes. The total contour length of the flagellum is fixed and is always given by L. Furthermore, we consider a sinusoidal flagellum at time t = 0 with beat shape $y(x)$ (orientation parallel to x-axis). Differential geometry implies

$$L = \int_0^{L_{eff}} dx \sqrt{1 + (\partial_x y)^2} \tag{S19}$$

For small beat amplitudes, the square root can be expanded to first order, so that

$$L = L_{eff} + \frac{1}{2}\int_0^{L_{eff}} dx\, (\partial_x y)^2 \tag{S20}$$

For a flagellum with a single wave length, the projected length of the flagellum is thus reduced from the full length with increasing beat amplitude changes as

$$\Delta L = L - L_{eff} = \pi^2 (A_b/L)^2 \tag{S21}$$

Moreover, the projected length of the flagellum has an influence on the rotational friction coefficient which is given by $\xi_{R,F} \sim L_{eff}^3$, analogous to a stiff rod where $\xi_{R,rod} \sim L^3$. Consequently, as increasing flexibility (Sp^4) leads to decrease of the beat amplitude, it implies an increase of the projected length, and thus of $\xi_{R,F}$, see Fig. S4.

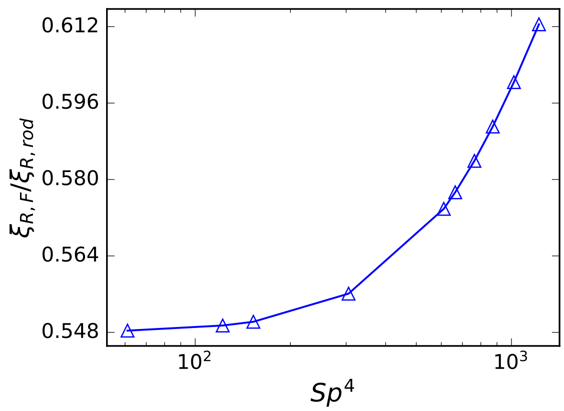

FIG. S4: **Rotational friction coefficient vs. Sp^4.** Variation of the ratio of rotation friction coefficients, $\xi_{R,F}/\xi_{R,rod}$, as a function of sperm number Sp^4. The coefficient increases with increasing Sp^4.

S6. MOVIE CAPTIONS

- **Movie M1** Reorientation of a symmetrically beating flagellum toward regions of higher viscosity, which demonstrates positive viscotaxis for $C_0L = 0.0$, $\tau/\tau_0 = 0.2$, $\alpha = 0.4$ and $\theta_{init} \approx 0.0$.

- **Movie M2** Linear motion of an asymmetric flagellum with small intrinsic curvature moving in a viscosity gradients with $C_0L = -0.0157$, $\tau/\tau_0 = 0.2$, $\alpha = 0.4$ and $\theta_{int} \approx 0.0$.

- **Movie M3** Trochoid-like motion perpendicular to the viscosity gradient of an asymmetric flagellum awith large intrinsic curvature, for $C_0L = -0.0628$, $\tau/\tau_0 = 0.2$, $\alpha = 0.4$ and $\theta_{int} \approx 0.0$.

[1] J. Gray and G. Hancock, J. Exp. Biol. **32**, 802 (1955).