Supplementary Information for Maximizing propulsive thrust of a driven filament at low Reynolds number via variable flexibility

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1. PROBLEM FORMULATION

We consider a slender filament of length L and uniform radius r such that $r \ll L$ and assume the filament is elastic and inextensible. The deformation of the filament is assumed to be confined to the x-y plane. We define the position vector of a material point on the filament neutral line relative to the laboratory frame as $\mathbf{x}(s,t)$, where s is the arclength along the filament with $s \in [0, L]$ and t represents time. It is convenient to describe the geometry by the local tangent angle made with the x axis as $\psi(s,t)$ such that $\mathbf{x}_s = \cos\psi \mathbf{e}_x + \sin\psi \mathbf{e}_y$, where the subscript s denotes the derivative with respect to s, namely $\mathbf{x}_s \equiv \partial_s \mathbf{x}$. See Fig. 1 in the main text for a schematic illustration.

The local unit tangent and normal vectors on the flagellum neutral line are defined as $\mathbf{t}$ and $\mathbf{n}$ respectively, with $\mathbf{t} = \mathbf{x}_s$. The local geometry is thus characterized by the Frenet-Serret formulas:

$$\mathbf{t}_s = \mathbf{x}_{ss} = \kappa \mathbf{n}, \quad \mathbf{n}_s = -\kappa \mathbf{t}, \tag{1.1}$$

where $\kappa = \|\mathbf{x}_{ss}\| = \psi_s$ is the local curvature.

We write the energy functional of the filament as [1, 2]

$$\mathcal{E} = \int_0^L \left[\frac{1}{2} A(s)\kappa^2 + \frac{1}{2}\sigma(\mathbf{x}_s^2 - 1) \right] \mathrm{d}s, \tag{1.2}$$

where $A(s) = E(s)I$ is the bending stiffness, with $E(s)$ the Young's modulus and I the second moment of inertia of the cross-section. The local inextensibility is enforced by the Lagrangian multiplier function $\sigma(s,t)$. We emphasize that in this work the bending stiffness is varying along the filament, $A = A(s)$, rather than uniform as has been done in previous studies. In the following, we closely follow the derivation given by Camalet and Jülicher [3] except that non-uniform stiffness distributions are allowed.

The variation of $\mathcal{E}$ with respect to a variation $\delta\mathbf{x}$ of the position vector $\mathbf{x}$ reads

$$\delta\mathcal{E} = \int_0^L \left[A\kappa\delta\kappa + \sigma \mathbf{x}_s \cdot \delta\mathbf{x}_s \right] \mathrm{d}s. \tag{1.3}$$

Using the relation $\delta\kappa = \delta\|\mathbf{x}_{ss}\| = \delta\left(\sqrt{\mathbf{x}_{ss}^2}\right) = \mathbf{n}\cdot\delta\mathbf{x}_{ss}$, we have

$$\delta\mathcal{E} = \int_0^L \left[A\kappa \mathbf{n}\cdot\delta\mathbf{x}_{ss} + \sigma \mathbf{x}_s \cdot \delta\mathbf{x}_s \right] \mathrm{d}s. \tag{1.4}$$

Upon integration by parts we obtain

$$\begin{aligned} \delta\mathcal{E} =& \Big[A\kappa\mathbf{n}\cdot\delta\mathbf{x}_s \Big]_{s=0}^{s=L} - \Big[\partial_s\left(A\kappa\mathbf{n}\right)\cdot\delta\mathbf{x} \Big]_{s=0}^{s=L} + \Big[\sigma\mathbf{x}_s\cdot\delta\mathbf{x} \Big]_{s=0}^{s=L} \\ &+ \int_0^L \partial_s \left[\partial_s(A\kappa\mathbf{n}) - \sigma\mathbf{x}_s \right]\cdot\delta\mathbf{x}\mathrm{d}s. \end{aligned} \tag{1.5}$$

The last term in Eq. (1.5) can be written as

$$\int_0^L \partial_s \left[\partial_s(A\kappa)\mathbf{n} - (A\kappa^2 + \sigma)\mathbf{t} \right]\cdot\delta\mathbf{x}\mathrm{d}s, \tag{1.6}$$

with the relation $\partial_s(A\kappa\mathbf{n}) = \partial_s(A\kappa)\mathbf{n} - A\kappa^2\mathbf{t}$. The elastic force density is therefore given by [4]

$$\mathbf{f}_{\text{elastic}} = -\partial_s\Big[\partial_s(A\kappa)\mathbf{n} - \tau\mathbf{t}\Big], \tag{1.7}$$

where we have defined $\tau = \sigma + A\kappa^2$, which represents the physical tension along the filament.

The boundary terms obtained from the variation $\delta\mathcal{E}$ are given by

$$\Big[A\kappa\mathbf{n}\cdot\delta\mathbf{x}_s\Big]_{s=0}^{s=L} + \Big[[-\partial_s(A\kappa)\mathbf{n} + \tau\mathbf{t}]\cdot\delta\mathbf{x}\Big]_{s=0}^{s=L}, \tag{1.8}$$

which represent external forces and torques applied at the two ends. Therefore, at the distal end ($s = L$),

$$T_{ext} = A\kappa, \quad \mathbf{F}_{ext} = \tau\mathbf{t} - \partial_s(A\kappa)\mathbf{n}, \tag{1.9}$$

and at the leading end ($s = 0$),

$$T_{ext} = -A\kappa, \quad \mathbf{F}_{ext} = -\tau\mathbf{t} + \partial_s(A\kappa)\mathbf{n}. \tag{1.10}$$

Since a slender filament is considered, the resistive force theory is employed to describe the hydrodynamics. The local viscous force distribution is given by

$$\mathbf{f}_{\text{vis}} = -(\xi_\perp\mathbf{nn} + \xi_\parallel\mathbf{tt})\cdot\mathbf{x}_t, \tag{1.11}$$

where the tangential and normal resistive coefficients are given by $\xi_\parallel$ and $\xi_\perp$ respectively. Neglecting the inertia of the filament, the elastic force has to balance the viscous force exerted by the surrounding fluids locally, i.e.

$$\mathbf{f}_{\text{vis}} + \mathbf{f}_{\text{elastic}} = \mathbf{0}. \tag{1.12}$$

Substituting the expressions of the viscous (Eq. 1.11) and elastic (Eq. 1.7) forces, the equation of motion is given by

$$\mathbf{x}_t = \frac{1}{\xi_\perp}\mathbf{n}\left(-\partial_s^2(A\psi_s) + \psi_s\tau\right) + \frac{1}{\xi_\parallel}\mathbf{t}\left(\psi_s\partial_s(A\psi_s) + \tau_s\right), \tag{1.13}$$

with $\kappa = \psi_s$. We employ the relations $\mathbf{t}_t = \psi_t\mathbf{n}$, $\mathbf{n}_s = -\psi_s\mathbf{t}$, and $\mathbf{t}_s = \mathbf{x}_{ss} = \psi_s\mathbf{n}$ and take the derivative of Eq. (1.13) with respect to s to obtain

$$\psi_t\mathbf{n} = \frac{1}{\xi_\perp}(-\psi_s\mathbf{t})\left(-\partial_s^2(A\psi_s) + \psi_s\tau\right) + \frac{1}{\xi_\parallel}\mathbf{t}\partial_s\left(\psi_s\partial_s(A\psi_s) + \tau_s\right) \tag{1.14}$$

$$+ \frac{1}{\xi_\perp}\mathbf{n}\partial_s\left(-\partial_s^2(A\psi_s) + \psi_s\tau\right) + \frac{1}{\xi_\parallel}\psi_s\mathbf{n}\left(\psi_s\partial_s(A\psi_s) + \tau_s\right). \tag{1.15}$$

From the tangential balance of Eq. 1.15, we obtain the governing equation for the tangent angleψ (s, t),

$$\psi_t = \frac{1}{\xi_\perp}\left(-\partial_s^3(A\psi_s) + \partial_s(\psi_s\tau)\right) + \frac{1}{\xi_\parallel}\psi_s\left(\psi_s\partial_s(A\psi_s) + \tau_s\right). \tag{1.16}$$

From the normal balance of Eq. 1.15, we obtain a differential equation for tension τ,

$$\tau_{ss} - \frac{\xi_\parallel}{\xi_\perp}\psi_s^2\tau = -\partial_s(\psi_s\partial_s(A\psi_s)) - \frac{\xi_\parallel}{\xi_\perp}\psi_s\partial_s^2(A\psi_s), \tag{1.17}$$

which equivalently enforces the inextensibility condition $\mathbf{x}_s\cdot\mathbf{x}_{st} = \mathbf{t}\cdot\mathbf{t}_t = 0$.

Eqs. (1.16) and (1.17) determine the filament dynamics. The filament shape can be recovered by integration:

$$\mathbf{x}(s, t) = \mathbf{x}(0, t) + \int_0^s [\cos\psi\mathbf{e}_x + \sin\psi\mathbf{e}_y]\mathrm{d}s', \tag{1.18}$$

where $\mathbf{x}(0, t)$ can be obtained from Eq. (1.13) by integration with respect to time and evaluating at $s = 0$.

2. BOUNDARY CONDITIONS

We consider the case of a clamped filament with sinusoidal displacement at one end ($s = 0$).

The clamped boundary condition is given by $\psi(0, t) = 0$ while the actuation boundary condition at $s = 0$,

$$y(0, t) = y_0 \sin \omega t, \tag{2.1}$$

is implemented through the equation of motion, Eq. (1.13), evaluated at $s = 0$:

$$y_0 \omega \cos \omega t \mathbf{e}_y = \frac{1}{\xi_\perp} \mathbf{n} \left(-\partial_{ss}(A\psi_s) + \psi_s \tau\right) + \frac{1}{\xi_\parallel} \mathbf{t} \left(\psi_s \partial_s (A\psi_s) + \tau_s\right). \tag{2.2}$$

The normal and tangential components of the equation, respectively, lead to the conditions

$$-\partial_s^2 (A\psi_s) + \psi_s \tau = \xi_\perp y_0 \omega \cos \omega t \cos \psi, \tag{2.3}$$
$$\psi_s \partial_s (A\psi_s) + \tau_s = \xi_\parallel y_0 \omega \cos \omega t \sin \psi, \tag{2.4}$$

evaluated at $s = 0$. With the clamped boundary condition,$\psi\ (0, t) = 0$, Eqs. 2.3 and 2.4 become

$$-\partial_s^2 (A\psi_s) + \psi_s \tau = \xi_\perp y_0 \omega \cos \omega t, \tag{2.5}$$
$$\psi_s \partial_s (A\psi_s) + \tau_s = 0. \tag{2.6}$$

The other end of the filament is free, and the force-free and torque-free conditions dictate that $\tau = 0$, $\psi_{ss} = 0$, and $\psi_s = 0$ at $s = L$.

To summarize, the boundary conditions at the two ends are:

$$\psi(0, t) = 0, \quad \left[\psi_s \partial_s (A\psi_s) + \tau_s\right]_{s=0} = 0, \quad \left[-\partial_s^2 (A\psi_s) + \psi_s \tau\right]_{s=0} = \xi_\perp y_0 \omega \cos \omega t, \tag{2.7}$$
$$\tau(L, t) = 0, \quad \psi_{ss}(L, t) = 0, \quad \psi_s(L, t) = 0. \tag{2.8}$$

The system of partial differential equations can now be solved with the above six boundary conditions.

3. DIMENSIONLESS GROUPS

We non-dimensionalize the equations by scaling length with L, time with ω^{-1}, and force with a characteristic viscous force magnitude $L^2 \xi_\perp \omega$. The resulting dimensionless groups (characteristic sperm number, dimensionless amplitude and drag anisotropy ratio) are given by

$$\mathrm{Sp}_0 = L \left(\frac{\xi_\perp \omega}{A_0}\right)^{1/4}, \quad \epsilon = \frac{y_0}{L}, \quad \gamma = \frac{\xi_\perp}{\xi_\parallel}, \tag{3.1}$$

where A_0 is a characteristic bending stiffness.

4. SMALL AMPLITUDE ASYMPTOTICS

We seek small-amplitude ($\epsilon \ll 1$) asymptotic solutions to the governing equations presented above.

A. Continuous stiffness distributions

In this section, we assume that $A(s)$ is continuous and calculate the leading order solution to the tangent angle and the propulsive force F_p. We assume regular perturbation expansions for ψ and τ:

$$= \epsilon \psi^{(1)} + \epsilon^2 \psi^{(2)} + \mathcal{O}(\epsilon^3),$$
$$\tau = \tau^{(0)} + \epsilon^2 \tau^{(2)} + \mathcal{O}(\epsilon^4), \tag{4.1}$$

where odd terms in τ vanish due to symmetry. Substituting the series into Eq. (1.17), we obtain $\partial_{ss}\tau^{(0)} = 0$ at order one. The corresponding boundary conditions can be readily obtained as $\tau^{(0)}(L, t) = 0$ and $\partial_s \tau^{(0)}(0, t) = 0$, and hence the solution is given by $\tau^{(0)}(s,t)=0$. As a result, tension is of $\mathcal{O}(\epsilon^2)$. Using Eq. (1.16), we obtain the leading order equation forψ ,

$$\psi_t^{(1)} + \frac{1}{\xi_\perp}\partial_s^3\left(A\psi_s^{(1)}\right) = 0, \tag{4.2}$$

with boundary conditions

$$\psi_{ss}^{(1)}(L,t)=0, \quad \psi_s^{(1)}(L,t)=0, \quad -\partial_s^2(A\psi_s^{(1)})(0,t)=\xi_\perp L\omega\cos\omega t, \quad \psi^{(1)}(0,t)=0. \tag{4.3}$$

Next, we calculate the time-averaged propulsive force

$$F_\mathrm{p} = -\left\langle \mathbf{e}_x \cdot \int_0^L \mathbf{f}_\mathrm{vis}\mathrm{d}s \right\rangle, \tag{4.4}$$

where the angle brackets denote time-averaging. We express F_p as a regular perturbation expansion,

$$F_\mathrm{p} = \epsilon^2 F_\mathrm{p}^{(2)} + \mathcal{O}(\epsilon^4), \tag{4.5}$$

where the odd terms in the series vanish due to the symmetry that the propulsive force should remain unchanged under the transformation $\epsilon \to -\epsilon$, or equivalently a phase shift of π of the actuation.

To leading order, the local tangent $\mathbf{t} \sim \mathbf{e}_x + \epsilon\psi^{(1)}\mathbf{e}_y$. Differentiating Eq. (1.18), we obtain the velocity vector as

$$\mathbf{u} \sim \left(\epsilon L\omega\cos\omega t + \epsilon\int_0^s \partial_t\psi^{(1)}\mathrm{d}s\right)\mathbf{e}_y. \tag{4.6}$$

The propulsive force then scales as

$$\begin{aligned}\mathbf{e}_x\cdot\mathbf{f}_\mathrm{vis} &= -\xi_\perp\mathbf{e}_x\cdot\mathbf{nn}\cdot\mathbf{u} - \xi_\parallel\mathbf{e}_x\cdot\mathbf{tt}\cdot\mathbf{u},\\ &\sim \epsilon^2(\xi_\perp-\xi_\parallel)\psi^{(1)}\left(L\omega\cos\omega t + \int_0^s\partial_t\psi^{(1)}\mathrm{d}s\right),\end{aligned} \tag{4.7}$$

where we can use Eq. (4.2) to evaluate the integral

$$\begin{aligned}\int_0^s \partial_t\psi^{(1)}\mathrm{d}s &= -\frac{1}{\xi_\perp}\left[\partial_s^2\left(A\psi_s^{(1)}\right) - \partial_s^2\left(A\psi_s^{(1)}\right)(0,t)\right]\\ &= -\frac{1}{\xi_\perp}\left[\partial_s^2\left(A\psi_s^{(1)}\right) + L\xi_\perp\omega\cos\omega t\right].\end{aligned} \tag{4.8}$$

As a result, the time-averaged propulsive force is given by

$$\langle\mathbf{e}_x\cdot\mathbf{f}_\mathrm{vis}\rangle \sim \epsilon^2\frac{\xi_\parallel-\xi_\perp}{\xi_\perp}\left\langle\psi^{(1)}\partial_s^2\left(A\psi_s^{(1)}\right)\right\rangle, \tag{4.9}$$

or equivalently,

$$F_\mathrm{p}^{(2)} = \frac{\xi_\perp-\xi_\parallel}{\xi_\perp}\left\langle\int_0^L \psi^{(1)}\partial_s^2\left(A\psi_s^{(1)}\right)\mathrm{d}s\right\rangle. \tag{4.10}$$

B. Segmented stiffness distributions

In this section, we consider segmented stiffness distribution (*i.e.* a step-function distribution), where we assume different but constant stiffnesses for the segments at the actuation end, A_1, and the distal end, A_2, with the ratio of stiffness denoted as $\beta = A_2/A_1$. The length of the segment at the driven end is given by αL with $\alpha \in [0,1]$.

For this segmented case, we can split the local tangent and tension into separate functions for the two segments. Denoting $\,_k^{(n)}$ as the tangent angle of the k-th ($k=1,2$) segment at $\mathcal{O}(\epsilon^n)$, we follow the same analysis in Sec. 4 A to obtain the governing equations for the tangent angle of the two segments:

$$\begin{aligned}\xi_\perp\partial_t\psi_1^{(1)} + A_1\partial_s^4\psi_1^{(1)} &= 0,\\ \xi_\perp\partial_t\psi_2^{(1)} + A_2\partial_s^4\psi_2^{(1)} &= 0.\end{aligned} \tag{4.11}$$

The corresponding boundary conditions are detailed in the main text.

The leading order velocity vector for the second segment reads

$$\mathbf{u}_2 \sim \left(\epsilon L\omega \cos\omega t + \epsilon \int_0^{\alpha L} \partial_t \psi_1^{(1)} \mathrm{d}s + \epsilon \int_{\alpha L}^{s} \partial_t \psi_2^{(1)} \mathrm{d}s \right) \mathbf{e}_y \tag{4.12}$$

and the expression for $\mathbf{u}_1$ takes the same form as Eq. (4.6). Evaluating the integrals

$$\int_0^{\alpha L} \partial_t \psi_1^{(1)} \mathrm{d}s + \int_{\alpha L}^{s} \partial_t \psi_2^{(1)} \mathrm{d}s = -\frac{1}{\xi_\perp} \left[A_1 \partial_s^3 \psi_1^{(1)}(\alpha L, t) + L\xi_\perp \omega \cos\omega t \right] - \frac{1}{\xi_\perp} \left[A_2 \partial_s^3 \psi_2^{(1)} - A_2 \partial_s^3 \psi_2^{(1)}(\alpha L, t) \right] \tag{4.13}$$

and employing the boundary condition $A_1 \partial_s^3 \psi_1^{(1)}(\alpha L, t) = A_2 \partial_s^3 \psi_2^{(1)}(\alpha L, t)$, we have

$$\mathbf{u}_2 \sim \left(\epsilon \frac{1}{\xi_\perp} A_2 \partial_s^3 \psi_2^{(1)} \right) \mathbf{e}_y. \tag{4.14}$$

As a result, we obtain the propulsive force for the segmented case as

$$F_{\mathrm{p}}^{(2)} = \frac{\xi_\perp - \xi_\parallel}{\xi_\perp} \left\langle A_1 \int_0^{\alpha L} {}_1^{(1)} \partial_s^3 \psi_1^{(1)} \mathrm{d}s + A_2 \int_{\alpha L}^{L} {}_2^{(1)} \partial_s^3 \psi_2^{(1)} \mathrm{d}s \right\rangle, \tag{4.15}$$

which upon integration by parts becomes

$$F_{\mathrm{p}}^{(2)} = \frac{\xi_\perp - \xi_\parallel}{\xi_\perp} \frac{1}{2} \left\langle A_1 \left(\partial_s \psi_1^{(1)} \right)^2 (0, t) - A_1 \left(\partial_s \psi_1^{(1)} \right)^2 (\alpha L, t) + A_2 \left(\partial_s \psi_2^{(1)} \right)^2 (\alpha L, t) \right\rangle. \tag{4.16}$$

5. NUMERICAL APPROACH

A. Numerical solution for continuous stiffness distributions

The ODE for $h(s)$, $i\mathrm{Sp}^4 h + (\mathcal{A} h_s)_{sss} = 0$, is a boundary value problem which is solved using Matlab's built-in `bvp4c` solver for a given stiffness profile. As a validation of the algorithm, the numerical results for both uniform ($\mathcal{A} = 1$) and two-segment stiffness distributions (approximated using hyperbolic tangent, see the main article, Sec. 3.3) match with the analytical solutions. Once the filament shape is obtained, the propulsive force can be evaluated by numerical integration here using Gauss-Legendre quadrature.

B. Numerical optimization

The optimization over polynomial and exponential stiffness distributions is performed using the `fmincon` solver in Matlab. For both linear and quadratic distributions, the optimization routine points to a limiting case where the boundary value problem (BVP) for $h(s)$ has a singular point at $s = 1$, *i.e.*, the stiffness at the free end goes to zero where the numerical solver itself cannot produce a solution. We then solved these two singular BVPs using the Matlab package `BVPSUITE` which can handle a singularity of the second kind [5–7].

[1] L. D. Landau and E. M. Lifshitz, *Theory of Elasticity*, 3rd ed. (Pergamon Press, Oxford, 1986).
[2] R. E. Goldstein and S. A. Langer, Phys. Rev. Lett. **75**, 1094 (1995).
[3] S. Camalet and F. Jülicher, New J. Phys. **2**, 24 (2000).
[4] Note that $\mathbf{f} = -\delta\mathcal{E}/\delta\mathbf{x}$.
[5] G. Kitzhofer, O. Koch, G. Pulverer, C. Simon, and E. Weinmüller, J. Numer. Anal. Indust. Appl. Math **5**, 113 (2010).
[6] F. R. De Hoog and R. Weiss, SIAM J. Numer. Anal. **13**, 775 (1976).
[7] F. R. de Hoog and R. Weiss, SIAM J. Math. Anal. **11**, 41 (1980).