Supporting information for: Optimization of chiral structures for micro-scale propulsion

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Shape optimization algorithm

The shape optimization algorithm that we use can be considered a type of gradient ascent method where the optimization variable is the shape. Thus, at each step of the optimization, we seek a perturbation field $\mathbf{V}$ that will deform the propeller to increase a specified objective functional. In our case, we find a $\mathbf{V}$ that results in a greater value of $U_z = \mathbf{U} \cdot \hat{\mathbf{z}}$ for the boundary value flow problem

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$$
\begin{aligned}
-\boldsymbol{\nabla} p + \eta \nabla^2 \mathbf{u} &= \mathbf{0} \\
\boldsymbol{\nabla} \cdot \mathbf{u} &= 0
\end{aligned}
\tag{S1}
$$

for fluid velocity field $\mathbf{u}$ and pressure p with

$$
\mathbf{u} = \mathbf{U} + \Omega_0 \hat{\mathbf{z}} \times \mathbf{x} \tag{S2}
$$

on the swimmer's surface. The surface of the swimmer's propeller is given by

$$
\mathbf{x}(t,\theta) = \mathbf{X}(t) + a_c(t)\left[\sin\theta \mathbf{n}_1 + \cos\theta \mathbf{n}_2\right] \tag{S3}
$$

with $t \in [-1,1]$, $\theta \in [0,2\pi]$, and $a_c(t) = a\sqrt{1-t^2}$. The components of $\mathbf{U}$ and the scalar Ω_0 are unknowns which we determine by imposing the following conditions for the total force and torque,

$$
\mathbf{F} = \int \mathbf{f} dS = \mathbf{0} \tag{S4}
$$

$$
\boldsymbol{\tau} = \int \mathbf{x} \times \mathbf{f} dS = \tau_0 \hat{\mathbf{z}} + \mathbf{T}. \tag{S5}
$$

where τ_0 is prescribed and $\mathbf{T}$ is unknown, but $\hat{\mathbf{z}} \cdot \mathbf{T} = 0$. As described in the text, this particular set of boundary conditions is taken to model the rotation and alignment of the swimmer by an applied magnetic field. The surface tractions are $\mathbf{f} = \boldsymbol{\sigma} \cdot \mathbf{n}$ where $\boldsymbol{\sigma} = -p\mathbf{I} + \eta(\boldsymbol{\nabla}\mathbf{u} + (\boldsymbol{\nabla}\mathbf{u})^T)$ is the Newtonian stress tensor and $\mathbf{n}$ is the unit normal to the swimmer's surface.

To determine this particular $\mathbf{V}$, we must first calculate the variation, δU_z, of U_z, with respect to an arbitrary perturbation field $\boldsymbol{\Phi}$. This is done using the machinery of shape differential calculus and the detailed calculation is presented in Walker et al.[S1] This calculation gives the expression

$$
\delta U_z(\boldsymbol{\Phi}) = \int (\boldsymbol{\Phi} \cdot \mathbf{n}) \mathbf{f} \cdot (\mathbf{I} - \mathbf{nn}) \cdot \mathbf{g} dS \tag{S6}
$$

where $\mathbf{g}$ are the surface tractions for an *adjoint* Stokes flow problem with $\mathbf{u} = \tilde{\mathbf{U}} + \tilde{\Omega}_0 \hat{\mathbf{z}} \times \mathbf{x}$ on the swimmer's surface, $\tilde{\mathbf{F}} = \tau_0 \hat{\mathbf{z}}$ and $\boldsymbol{\tau} = \tilde{\mathbf{T}}$ with $\tilde{\mathbf{T}} \cdot \hat{\mathbf{z}} = 0$. As with the original Stokes flow, the components of $\tilde{\mathbf{U}}$, the scalar $\tilde{\Omega}_0$, and two components of $\tilde{\mathbf{T}}$ are unknowns. In our optimizations, we consider perturbations $\boldsymbol{\phi}$ of the centerline, but we need $\boldsymbol{\Phi} \cdot \mathbf{n}$ on the swimmer's surface to evaluate the shape derivative. Using the equation for the surface, S3, this can be found using the following formula

$$\boldsymbol{\Phi} \cdot \mathbf{n} = \boldsymbol{\phi} \cdot \mathbf{n} + a_c(t)(\cos\theta \delta \mathbf{n}_1 + \sin\theta \delta \mathbf{n}_2) \cdot \mathbf{n} \tag{S7}$$

where $\delta \mathbf{n}_1 = \mathbf{n}_2 \times \delta \mathbf{t}$ and $\delta \mathbf{n}_2 = -\mathbf{n}_1 \times \delta \mathbf{t}$. The variation $\delta \mathbf{t}$ of the centerline tangent is completely determined by $\boldsymbol{\phi}$ and given by

$$\delta \mathbf{t} = (\mathbf{I} - \mathbf{t}\mathbf{t}) \cdot \frac{d\boldsymbol{\phi}}{ds} \tag{S8}$$

where s is the arclength.

In the main text, we described the centerline $\mathbf{X}$ in terms of the arclength $s \in [-L, L]$. In the optimizations, however, we utilize a more general parametization, $\mathbf{X}(t)$ with $t \in [-1, 1]$, see S3. We then impose the local inextensibility condition, $|d\mathbf{X}/dt| = L$ using Lagrange multipliers, λ. Specifically, we consider the integral form of this condition,

$$L = \int_{-1}^{1} \mu(|\mathbf{X}(t)| - |\mathbf{X}_0(t)|)dt = 0 \tag{S9}$$

for all choices of μ, where $\mathbf{X}_0(t)$ is the reference centerline. The shape derivative of this functional is

$$\delta L(\mu, \phi) = \int_{-1}^{1} \mu(\mathbf{t} \cdot \frac{d\phi}{ds})dt. \tag{S10}$$

Using these expressions and following Walker et al.,[S2] we establish the variational formulation for obtaining an ascent perturbation of the shape at each step of the optimization. Find the perturbation $\mathbf{V}$ and Lagrange multiplier λ such that

$$\langle \mathbf{V}, \boldsymbol{\phi} \rangle + \delta L(\boldsymbol{\phi}, \lambda) \quad = \quad \delta U_z(\boldsymbol{\Phi}) \tag{S11}$$

$$\delta L(\mathbf{V}, \mu) = -L(\mu) \tag{S12}$$

for all $\boldsymbol{\phi}$ and μ. Here, we use the inner product

$$\langle \mathbf{q}(t), \mathbf{r}(t) \rangle = \int \mathbf{q} \cdot \mathbf{r} dt + \int \frac{d\mathbf{q}}{dt} \cdot \frac{d\mathbf{r}}{dt} dt + \int \frac{d^2\mathbf{q}}{dt^2} \cdot \frac{d^2\mathbf{r}}{dt^2} dt \tag{S13}$$

where the integrals are defined over the centerline. This inner product ensures the shape remains smooth. In the numerical implementation, we consider $\mathbf{V}$ given by cubic splines defined over N_{seg} segments of the centerline. We take λ to be piecewise constant over these segments, which implies that the length of each segment is kept constant during the optimization. It can be proven[S1] that the resulting $\mathbf{V}$ is an ascent perturbation and, consequently, will morph the swimmer into a shape with a higher speed.

Boundary integral equations

In order to determine the variations in the functionals with respect to changes in the swimmer shape, we must compute the tractions on the body for the original and adjoint Stokes flow problems. To do this for the complex swimmer geometries, we use a second-kind boundary integral formulation for the tractions on a rigid body. This formulation avoids the numerical ill-conditioning associated with the standard first-kind boundary integral equation and allows us to compute the functional variations with fidelity necessary to resolve the ascent direction in the shape space. Using index notation, this integral equation for the tractions is

$$\begin{aligned} U_i + (\boldsymbol{\Omega} \times \mathbf{x})_i &= \frac{1}{2\eta} f_i(\mathbf{x}) \\ &\quad + n_k(\mathbf{x}) \int_D T_{ijk}(\mathbf{y} - \mathbf{x}) f_j(\mathbf{y}) dS_{\mathbf{y}} + \mathscr{V}_i^T[\mathbf{f}](\mathbf{x}). \end{aligned} \tag{S14}$$

where the integrals are taken over the surface of the swimmer,

$$T_{ijk}(\mathbf{x}-\mathbf{y}) = \frac{3}{4\pi\eta}\frac{(x_i-y_i)(x_j-y_j)(x_k-y_k)}{|\mathbf{x}-\mathbf{y}|^5}, \tag{S15}$$

and $\mathscr{V}_i^T[\mathbf{f}](\mathbf{x})$ is the adjoint completion flow. $\mathscr{V}_i^T[\mathbf{f}](\mathbf{x})$ is given by

$$\begin{aligned}\mathscr{V}_i^T[\mathbf{f}](\mathbf{x}) &= \int_D G_{ji}(\mathbf{y}-\mathbf{X}(\mathbf{x}))f_j(\mathbf{y})dS_{\mathbf{y}} \\ &\quad +\varepsilon_{ijk}(x_k-X_k(\mathbf{x}))\int_D f_l(\mathbf{y})R_{lj}(\mathbf{y}-\mathbf{X}(\mathbf{x}))dS_{\mathbf{y}}\end{aligned} \tag{S16}$$

and is based on a linear combination of Stokeslets

$$G_{ij}(\mathbf{x}) = \frac{1}{8\pi\eta}\left(\frac{\delta_{ij}}{|\mathbf{x}|}+\frac{x_ix_j}{|\mathbf{x}|^3}\right) \tag{S17}$$

and rotlets

$$R_{ij}(\mathbf{x}) = \frac{1}{8\pi\eta}\frac{\varepsilon_{ijk}x_k}{|\mathbf{x}|^3} \tag{S18}$$

distributed at the set of points $\mathbf{X}$ along the centerline of the body.

Before discretizing, we first remove the $1/r$ divergence in the integrand on the right hand side of S14 by rewriting the first two terms

$$\mathscr{I}_i(\mathbf{x}) = \frac{1}{2\eta}f_i(\mathbf{x})+n_k(\mathbf{x})\int_D T_{ijk}(\mathbf{y}-\mathbf{x})f_j(\mathbf{y})dS_{\mathbf{y}} \tag{S19}$$

as

$$\mathscr{I}_i(\mathbf{x}) = \int_D T_{ijk}(\mathbf{y}-\mathbf{x})\left(f_j(\mathbf{y})n_k(\mathbf{x})+f_j(\mathbf{x})n_k(\mathbf{y})\right)dS_{\mathbf{y}}. \tag{S20}$$

We then approximate the integrals to second-order using the trapezoidal rule where the contribution from the source whose location coincides with the field point is removed from the sum. The details regarding the discretization scheme and a verification of the method can be found in Keaveny et al.[S3]

Swimmer parametrization

For our examination of the propeller cross-section orientation, we utilize the following parametrization of the swimmer surface

$$\mathbf{x}(s,\theta) = \mathbf{X}(s) + r_n(s)\sin\theta\mathbf{n}_1 + r_b(s)\cos\theta\mathbf{n}_2. \tag{S21}$$

For the centerline, we take

$$\mathbf{X}(s) = \int_{-L}^{s} d\mathbf{X}/ds' ds' \tag{S22}$$

where

$$\frac{d\mathbf{X}}{ds} = \hat{\mathbf{t}}_{hel}(L)\chi(L) + \int_{-L}^{s} \chi(s')\frac{d^2\mathbf{X}_{hel}}{ds'^2}ds'. \tag{S23}$$

The function $\chi(s) = \left[1 - \mathrm{erf}((s-s_0)/(\sqrt{2}\sigma))\right]/2$ governs the transition between the flat head and tail regions. To match the head size in the Zhang et al. experiments, we set $s_0/L = 1 - 9.0/54.2$ and take $\sigma/L = 0.02$. The unit vectors, $\mathbf{n}_1$ and $\mathbf{n}_2$ are normal to the centerline tangent $\mathbf{t}$ and related to the Serret-Frenet normal $\mathbf{N}$ and binormal $\mathbf{B}$ through

$$\mathbf{n}_1 = \mathbf{N}\cos\Gamma(s) + \mathbf{B}\sin\Gamma(s) \tag{S24}$$

$$\mathbf{n}_2 = \mathbf{B}\cos\Gamma(s) - \mathbf{N}\sin\Gamma(s) \tag{S25}$$

where $\Gamma(s) = \gamma\left[1 - \mathrm{erf}((s-s_1)/(\sqrt{2}\sigma))\right]/2$ with γ being the rotation angle in the propeller. We also set $s_1/L = 1 - 11.0/54.2$ and $\sigma/L = 0.02$. The vector $\mathbf{n}_2$ serves as the long axis of the propeller cross-section and has radius $r_b(s) = a_b(c_1 - c_2\chi(s))(1-s^8)^{1/8}$ with $a_b/L = 1/27$. The constants $c_1 = 2.75$ and $c_2 = 1.75$ set the magnitude of the r_b in the head and propeller sections. Finally, for the short axis of the propeller cross-section, $\mathbf{n}_1$, we set its radius to be $r_n(s) = r_b(s)/4$.

Mobility matrices of optimal shape

Here, we provide the mobility coefficients for the swimmer shapes shown in Figures 4 and 5. Given the helical symmetry of the swimmers, we take the approximation $U_z = M_A F_z + M_B \tau_z$ and $\Omega_z = M_B F_z + M_D \tau_z$. We obtain the values of M_A, M_B, and M_D by solving the Stokes equations subject to the boundary conditions used in our shape optimization routine. The resistance, or drag coefficients can be found by inverting the linear relations. For the swimmers shown in Figure 4, the mobility coefficients are provided in Table S1 The entries for the swimmers in Figure 5 with

Table S1: Mobility coefficients for the swimmers shown in Figure 4 in the text.

L/R	$\eta R M_A$	$\eta R^2 M_B$	$\eta R^3 M_D$
GF	2.53×10^{-2}	4.74×10^{-4}	1.07×10^{-2}
OPT_1	2.24×10^{-2}	1.17×10^{-3}	4.77×10^{-3}
OPT_2	3.37×10^{-2}	2.21×10^{-3}	1.33×10^{-2}

$a/R = 0.4$ are given in Table S2. while those for $a/R = 0.2$ are in Table S3 It is interesting, and

Table S2: Mobility coefficients for the swimmers shown in Figure 5 in the text with $a/R = 0.4$

L/R	$\eta R M_A$	$\eta R^2 M_B$	$\eta R^3 M_D$
2	4.10×10^{-2}	1.22×10^{-3}	1.95×10^{-2}
4	3.37×10^{-2}	1.74×10^{-3}	1.18×10^{-2}
6	2.78×10^{-2}	1.62×10^{-3}	7.60×10^{-3}
8	2.41×10^{-2}	1.42×10^{-3}	5.85×10^{-3}

Table S3: Mobility coefficients for the swimmers shown in Figure 5 in the text with $a/R = 0.2$

L/R	$\eta R M_A$	$\eta R^2 M_B$	$\eta R^3 M_D$
2	4.37×10^{-2}	1.48×10^{-3}	2.27×10^{-2}
4	3.61×10^{-2}	2.18×10^{-3}	1.58×10^{-2}
6	3.08×10^{-2}	2.12×10^{-3}	1.19×10^{-2}
8	2.73×10^{-2}	1.93×10^{-3}	8.27×10^{-3}

perhaps useful, to note that the mobility coefficients[S4] M_A and M_D can be estimated using the expressions for prolate spheroids

$$M_A^{PS} = \frac{(1+\varepsilon^2)\mathscr{L} - 2\varepsilon}{16\pi\eta\zeta_{eff}R\varepsilon^3} \tag{S26}$$

$$M_D^{PS} = \frac{6\varepsilon - 3(1-\varepsilon^2)\mathscr{L}}{32\pi\eta\zeta_{eff}^3 R^3\varepsilon^3(1-\varepsilon^2)} \tag{S27}$$

where $\zeta_{eff} = L/R$, $\varepsilon = (1-\zeta_{eff}^{-2})^{1/2}$, and $\mathscr{L} = \log((1+\varepsilon)/(1-\varepsilon))$. These expressions yield those values give in Table S4 which are comparable to the values for the swimmer shapes.

Table S4: Mobility coefficients for the prolate spheroids.

L/R	$\eta R M_A$	$\eta R^3 M_D$
2	4.41×10^{-2}	2.47×10^{-2}
4	3.32×10^{-2}	1.38×10^{-2}
6	2.70×10^{-2}	9.52×10^{-3}
8	2.29×10^{-2}	7.25×10^{-3}

References

(S1) Walker, S. W.; Keaveny, E. E. *in preparation*

(S2) Walker, S. W.; Shelley, M. J. *Journal of Computational Physics* **2010**, *229*, 1260 – 1291.

(S3) Keaveny, E. E.; Shelley, M. J. *J. Comput. Physics* **2011**, *230*, 2141–2159.

(S4) Kim, S.; Karrila, S. J. *Microhydrodynamics: Principles and Selected Applications*; Dover Publications, Inc., 2005.