Appendix A. Swimming motion and shape parametrization

The swimming motion chosen here is based on Carling *et al.* (1998); Kern & Koumoutsakos (2006), and is defined by an explicit equation for the lateral displacement of the midline $y_s(s,t)$ in a local frame of reference:

$$y_s(s,t) = 0.125L\frac{0.03125 + \dfrac{s}{L}}{1.03125}\sin\left[2\pi\left(\frac{s}{L} - \frac{t}{\mathcal{T}}\right)\right], \tag{A 1}$$

where L is the swimmer's length, s is the arc length of the mid-line of the body ($0 \leqslant s \leqslant L$), t is the time, and $\mathcal{T}$ the swimming period.

Since our swimmers start from rest, we ramp up their motion by a cubic function during the first cycle, ensuring a smooth transition between the state of rest and the desired motion.

As indicated in the main text, our shape parametrization is capable of representing for a large variety of shapes with only 10 parameters. This flexibility is highlighted in figure 1, where several shapes generated during the initial phase of our optimization are presented.

Appendix B. Details on the efficiency definition and computation

Here we further detail the definition of efficiency used in this work, and how the relevant quantities are extracted from the numerical simulations. For completeness, we repeat the definition given in the main text:

$$f_{\text{eff}} = -\frac{E_{\text{useful}}}{E_{\text{input}} + E_{\text{useful}}} = -\frac{m\bar{U}^2/2}{\left(\int_{5\mathcal{T}}^{6\mathcal{T}} P_{\text{input}}(t)\,\mathrm{d}t\right) + m\bar{U}^2/2}, \tag{B 1}$$

where m is the mass of the swimmer and $\bar{U}$ is the average forward velocity, defined in the main text of this work. P_{input} is the total instantaneous power delivered to the fluid, which accounts for the rate of change of kinetic energy and dissipation due to viscous stresses. In the following we wish to clarify the definition and computation of P_{input}.

B.1. *Definition of input power*

We consider the total instantaneous power delivered to the flow as:

$$P_{\text{input}} = \int_{\partial\Omega} (\mathbf{n}\cdot\boldsymbol{\sigma}\cdot\mathbf{u})\,\mathrm{d}S, \tag{B 2}$$

where $\partial\Omega$ is the surface of our body.

Applying Gauss' theorem to this integral gives:

$$P_{\text{input}} = \int_{\Sigma\setminus\Omega} (\nabla\cdot\boldsymbol{\sigma}\cdot\mathbf{u})\,\mathrm{d}V \tag{B 3}$$

$$= \int_{\Sigma\setminus\Omega} (\mathbf{u}(\nabla\cdot\boldsymbol{\sigma}) + \boldsymbol{\sigma} : \nabla\mathbf{u})\,\mathrm{d}V, \tag{B 4}$$

where Σ covers the entire domain and Ω covers only the support of the body. The first term of the second equation can be obtained by dotting the Navier-Stokes equation with the velocity vector, whereas for the second term we can substitute the definition of the stress tensor $\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\tau}$:

$$P_{\text{input}} = \int_{\Sigma\setminus\Omega} \left(\rho\frac{\mathrm{D}}{\mathrm{D}t}\frac{u^2}{2} - p\nabla\cdot\mathbf{u} + \boldsymbol{\tau} : \nabla\mathbf{u}\right)\,\mathrm{d}V, \tag{B 5}$$

where $u^2 = \mathbf{u} \cdot \mathbf{u}$. Using the incompressibility condition of our fluid, $\nabla \cdot \mathbf{u} = 0$, and the Newtonian shear stress tensor $\boldsymbol{\tau} = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ with μ the kinematic viscosity, we finally get:

$$P_{\text{input}} = \frac{\mathrm{d}}{\mathrm{d}t} \int_{\Sigma \setminus \Omega} \rho \frac{u^2}{2} \, \mathrm{d}V + \mu \int_{\Sigma \setminus \Omega} \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) : \nabla \mathbf{u} \, \mathrm{d}V. \tag{B 6}$$

This is the formulation used in our work to compute the input power.

B.2. *Computation of input power*

As detailed in the main text of this work, our numerical method is based on the vorticity-velocity formulation of the Navier-Stokes equations with free-space boundary conditions. This means that the velocity field, which physically spans the entire free-space, is not entirely contained within the computational domain. Consequently, the evaluation of the input power P_{input} (Eq. B 6) is non trivial.

Concerning the first term in equation (B 6) we note that, for a divergence-free velocity field, the following kinematic identity holds:

$$\int_{\Sigma \setminus \Omega} \mathbf{u} \cdot \mathbf{u} \, \mathrm{d}V = \int_{\Sigma \setminus \Omega} \Psi \cdot \boldsymbol{\omega} \, \mathrm{d}V. \tag{B 7}$$

Here Ψ is the streamfunction, defined as the solution of the Poisson equation

$$\nabla^2 \Psi = -\boldsymbol{\omega}, \tag{B 8}$$

hence $\mathbf{u} = \nabla \times \Psi$. The integral on the right-hand side of equation (B 7) can be computed in Fourier space (Chatelain & Koumoutsakos 2010) from a compact vorticity field, and thus the kinetic energy in a domain with free-space boundary conditions can be computed given only the vorticity field. In the current case, due to the deformation velocity field of the swimmer, the velocity field inside the body is in general not divergence free, and therefore this approach needs to be amended. The velocity field can be expressed via the Helmholtz-Hodge decomposition

$$\mathbf{u} = \nabla \times \Psi + \nabla \phi, \tag{B 9}$$

with

$$\nabla^2 \phi = \nabla \cdot \mathbf{u}, \tag{B 10}$$

where the field $\nabla \cdot \mathbf{u}$ is non-zero only within the swimmer's support. The integral equation for the kinetic energy then expands into three contributions:

$$\int_{\Sigma \setminus \Omega} \mathbf{u} \cdot \mathbf{u} \, \mathrm{d}V = \int_{\Sigma \setminus \Omega} \{ (\nabla \times \Psi \cdot \nabla \times \Psi) + (\nabla \phi \cdot \nabla \phi) + 2(\nabla \times \Psi \cdot \nabla \phi) \} \, \mathrm{d}V. \tag{B 11}$$

All three of these integrals can be computed in Fourier space based on compact fields in physical space ($\boldsymbol{\omega}$ and $\nabla \cdot \mathbf{u}$), and the sum of these three integrals results in the total kinetic energy in the domain. Since we need to compute the kinetic energy only in the fluid domain, we subtract the kinetic energy within the solid shape, easily calculated in physical space, from this sum. Finally, the derivative of the integral is computed with a first order finite difference technique applied between two subsequent timesteps.

The second integral in Eq. B 6 represents the viscous dissipation term. We argue that due to the low Reynolds number and the corresponding strong decay of the vorticity away from the swimmer, the velocity gradients $\nabla \mathbf{u}$ outside our domain give negligible contributions to the integral, and can be ignored in the computation for the input power.

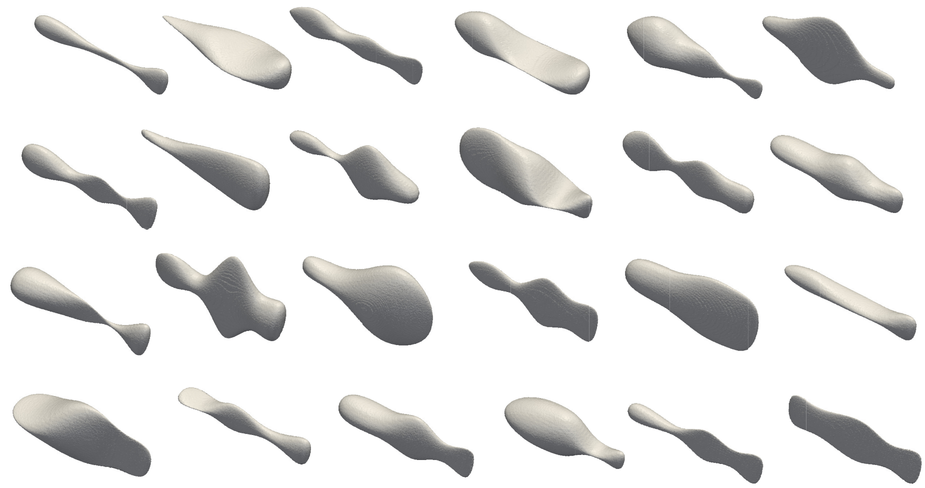

Figure 1: Perspective view of several shapes generated via the B-spline parametrization proposed in this work. For every shape, the head is in the top left, the tail is in the bottom right.

The convergence of this approach has been verified through successive domain increases and the assumptions were found to have a negligible influence on the value of the computed efficiency.

REFERENCES

Carling, J., Williams, T. L. & Bowtell, G. 1998 Self-propelled anguilliform swimming: Simultaneous solution of the two-dimensional Navier-Stokes equations and newton's laws of motion. *Journal of Experimental Biology* **201** (23), 3143–3166.

Chatelain, P. & Koumoutsakos, P. 2010 A fourier-based elliptic solver for vortical flows with periodic and unbounded directions. *Journal of Computational Physics* **229** (7), 2425 – 2431.

Kern, S. & Koumoutsakos, P. 2006 Simulations of optimized anguilliform swimming. *Journal of Experimental Biology* **209** (24), 4841–4857.