Parametric shape optimization of flagellated microswimmers using Bayesian techniques

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Understanding and optimizing the design of helical microswimmers is crucial for advancing their application in various fields.The **Boundary Element Method** (BEM) is used to simulate the dynamic [1]. Due to the complexity of our model, we focus on **parametric shape optimization**. We employ the **Free-Form Deformation** (FFD) technique [2], which provides a sufficiently complex admissible shape space. This is integrated with the **Scalable Constrained Bayesian Optimization** (SCBO) method [3], ideal for high-dimensional constrained optimization problems.

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Flagella geometry of microswimmers

The swimmer, denoted by S, is composed of a head H and a set of n_f of flagella, i.e. $S = H \bigcup_{i=1}^{n_F} F_i$. Each flagellum F_i is a tube of radius r with a centerline of total length L.

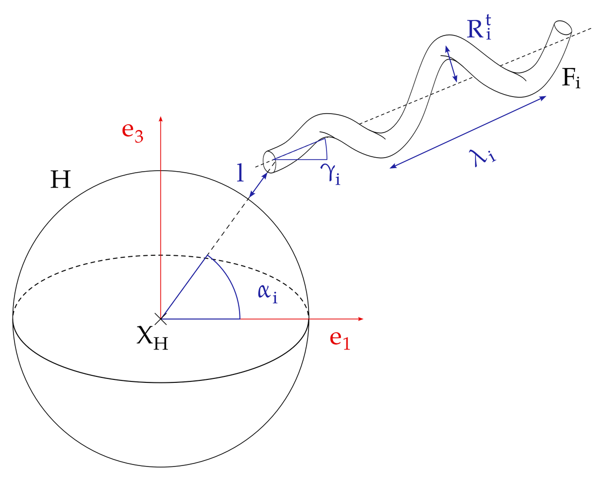

Figure 1. Schematic of microswimmers represented by an arbitrary flagellum.

	Fixed parameters		Optimized parameters
r	Radius of the flagella	R^t	Amplitude
L	Total length	λ	Wavelength
l	Junction distance	$\alpha, \beta, \gamma, \delta$	Angles for position and orientation

Table 1. Fixed and optimized parameters of flagella.

Head geometry of microswimmers

The head is obtained as the image of the **Free-Form-Deformation** (FFD) map T applied to the unit sphere, where **control points** $P \in \mathbb{R}^{3M}$ are shifted by a vector $\mu \in \mathbb{R}^{3M}$,

$$T : D \times \mathbb{R}^{3\times M} \to D(\mu)$$
$$(\Theta, \mu) \mapsto \left(\psi^{-1} \circ \hat{T} \circ \psi\right)(\Theta, \mu),$$

where $\hat{T}(\cdot) = \sum_{i=0}^{J}\sum_{j=0}^{J}\sum_{k=0}^{K} b_{i,j,k}^{I,J,K}(\cdot)(P+\mu)_{i,j,k}$ and $b_{i,j,k}^{I,J,K}(\cdot)$ is the tensor products of **Bernstein polynomials**.

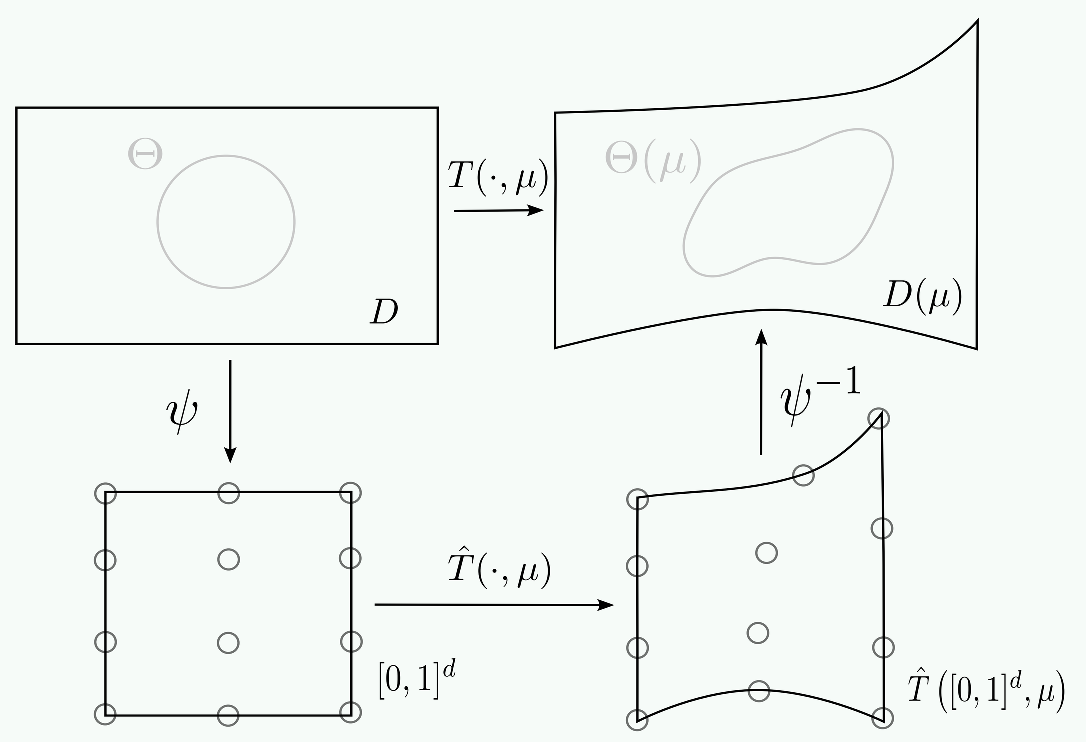

Figure 2. Illustration of the FFD method deforming a domain D containing a Θ shape via a μ vector using the T map.

Dynamic of microswimmers

Due to the **low Reynolds number** in microswimmer dynamics, the fluid behavior is governed by the **Stokes** equations given by

$$\begin{cases} -\mu\Delta u + \nabla p = 0 & \text{in } \mathbb{R}^3 \setminus S, \\ \nabla \cdot u = 0 & \text{in } \mathbb{R}^3 \setminus S, \\ u = U + \Omega \wedge (x - x^H) & \text{on } \partial H, \\ u = U + \Omega \wedge (x - x^H) + \omega e_1^{F_i} \wedge (x - x^{F_i}) & \text{on } \partial F_i, \\ \|u\|, p \to 0 & \text{as } x \to +\infty, \end{cases}$$

for all $i \in \{1, \ldots, n_F\}$.

Parameter	Description
u, p	Velocity and pressure of the fluid
U, Ω	Translational and angular velocities of the swimmer
$\omega = -2\pi \text{rad.s}^{-1}$	Angular velocity of the flagella
$e_1^{F_i}$	Directional axes of the flagellum F_i
x^{F_i}, x^H	Junction point of the flagellum F_i and head center of mass

Table 2. Parameters of the Stokes PDE.

Boundary Element Method

1. **Green tensor kernel** : $u(y) = -\int_{\partial S} G(x,y)\sigma(u,p)(x)n(x)dx$ for all y in $\mathbb{R}^3$.
2. **Self-propulsion** : $\int_{\partial S}\sigma(u,p)(x)n(x)dx = 0$, $\int_{\partial S}\sigma(u,p)(x)n(x)\wedge(x - x^H)dx = 0$.
3. $\mathbb{P}^1$ **finite element space** of ∂S.

Shape optimization problem

- Admissible shapes : $\mathcal{S}_{ad} = \mathcal{H}_{ad}^{\varepsilon} \times \mathcal{F}_{ad}^{\mathcal{P}}$
- Admissible flagella : $\mathcal{F}_{ad}^{\mathcal{P}} = \{\, F \subset \mathbb{R}^3 \mid (\lambda, R^t, \alpha, \gamma, \beta, \delta) \in \mathcal{P}$ and $|F| = |F^0| \,\}$ where $\mathcal{P}$ is a compact set.
- Admissible heads : $\mathcal{H}_{ad}^{\varepsilon} = \left\{H = T(H^0, \mu) \mid \mu \in \mathcal{V} \text{ and } ||H| - |H^0|| \leq \varepsilon \right\}$ where $\mathcal{V}$ is a sufficiently small closed set around the control points to **prevent mesh collapse**.
- Cost functions : J_1 for the **mean velocity** and J_2 for the **mean efficiency** along e_1,

$$J_1(S) = -\frac{\bar{U}_1(S)}{\bar{U}_1^0} \quad \text{and} \quad J_2(S) = -\frac{\bar{U}_1(S)}{\bar{U}_1^0} \times \frac{\bar{P}^0}{\bar{P}(S)}.$$

Finally, the optimization problem for $i \in \{1,2\}$ is formulated as $\inf_{S \in \mathcal{S}_{ad}} J_i(S)$.

High dimensional Bayesian optimization method

Gaussian Process (GP) is used to model costly functions from a given dataset D_n.

- Prior: $J \sim \mathcal{GP}(0,k)$
- Posterior: $J \mid D_n \sim \mathcal{GP}(\mu, \Sigma)$

with
$$\begin{cases} \mu(x) = K(x, X_n)K_n^{-1}Y_n, \\ \Sigma(x) = K(x,x) - K(x,X_n)K_n^{-1}K(X_n,x), \\ (K(X,X'))_{i,j} = k(X_i, X_j') \text{ and } K_n = K(X_n, X_n). \end{cases}$$

The SCBO method is based on the **trust region** approach, which outperforms conventional Bayesian Optimization (BO).

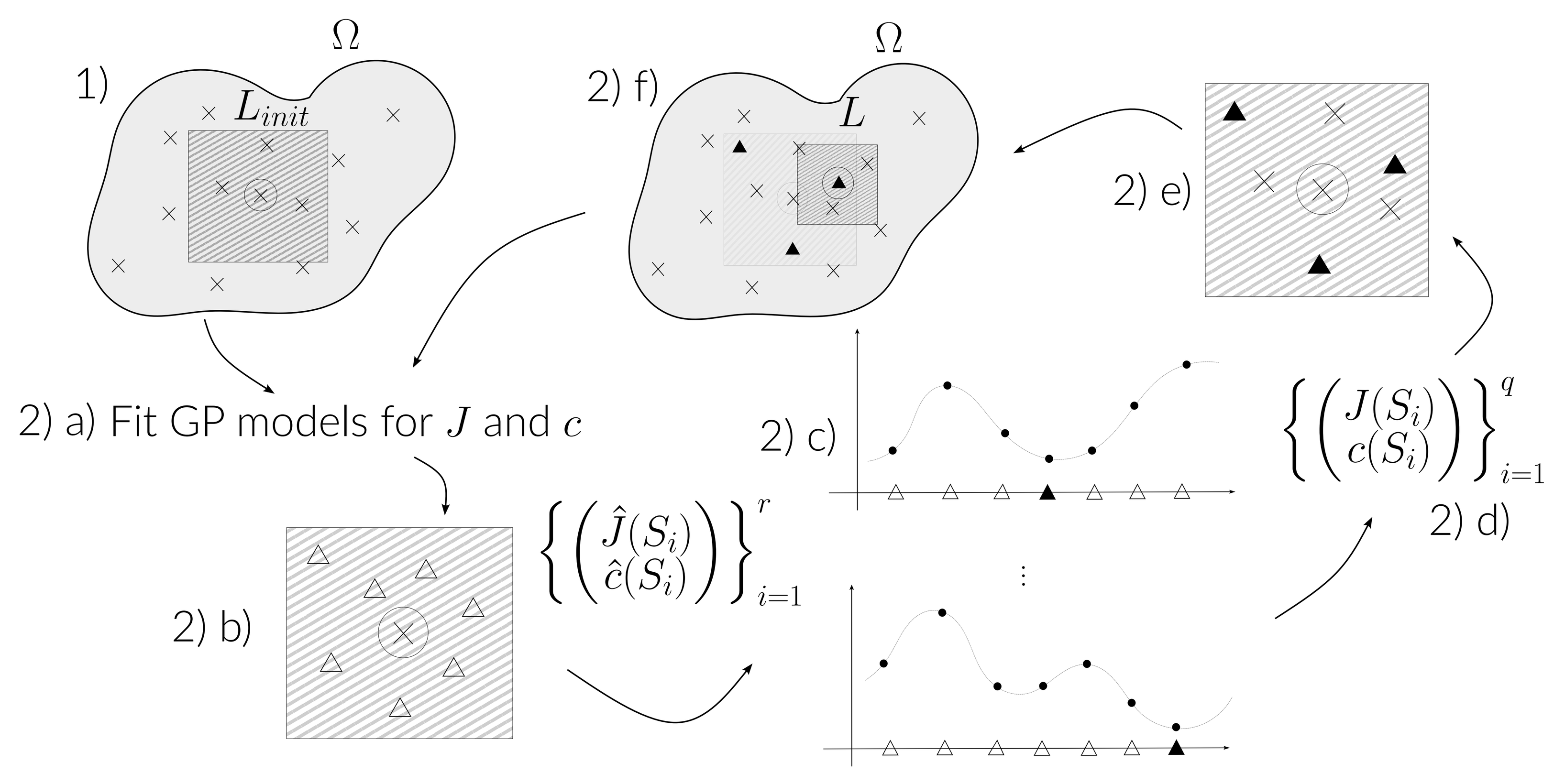

Figure 3. Illustration of the Scalable Constrained Bayesian Optimization (SCBO) method developed in [3].

Results

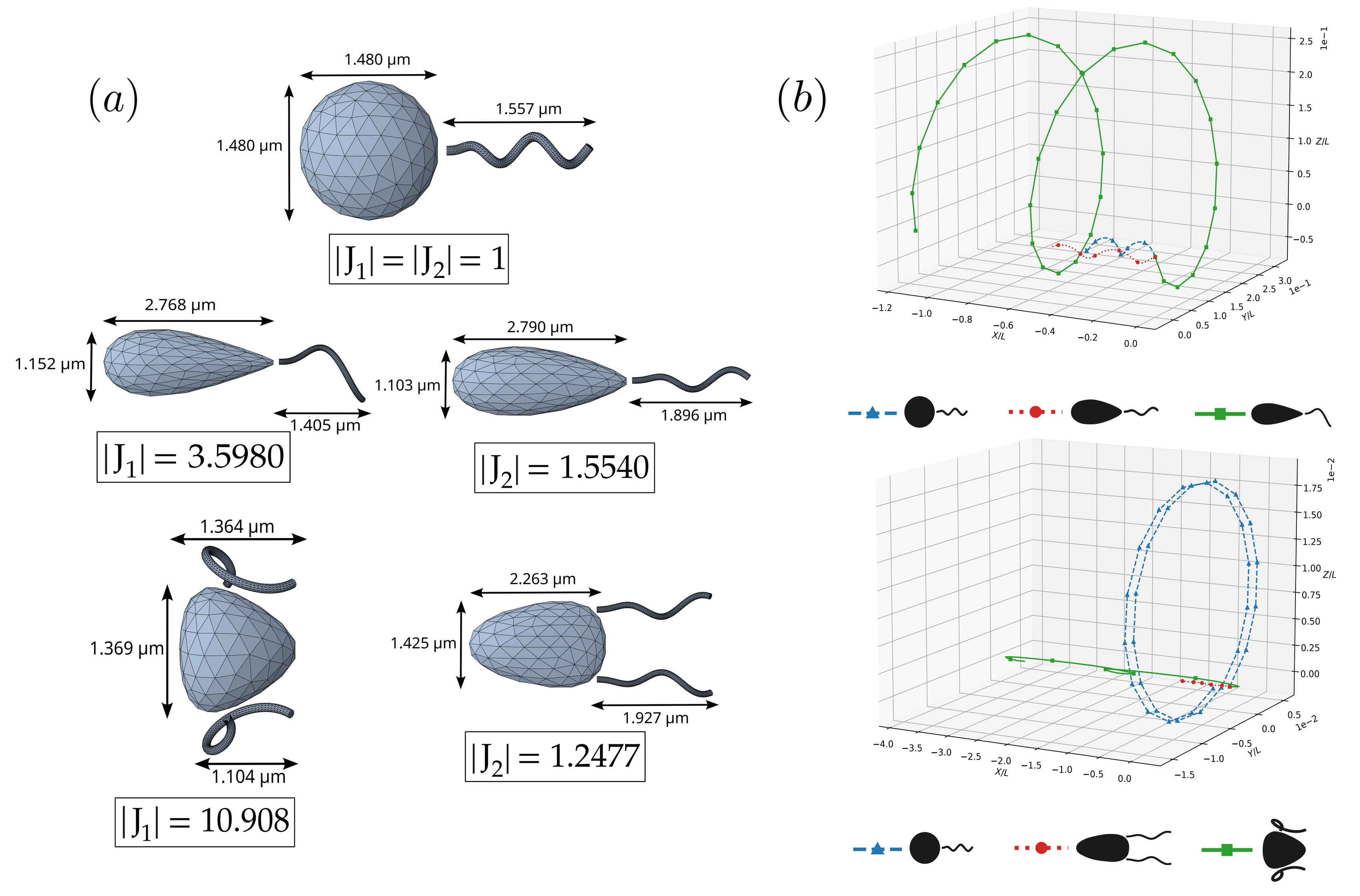

Figure 4. (a) Reference swimmer and the best swimmers. (b) Center of mass trajectories.

Video

References

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