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Bacteria-inspired robotic propulsion from bundling of soft helical filaments at low Reynolds number†

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The bundling of flagella is known to create a “run” phase, where the bacteria moves in a nearly straight line rather than making changes in direction. Historically, mechanical explanations for the bundling phenomenon intrigued many researchers, and significant advances were made in physical models and experimental methods. Contributing to the field of research, we present a bacteria-inspired centimeter-scale soft robotic hardware platform and a computational framework for a physically plausible simulation model of the multi-flagellated robot under low Reynolds number ($\sim 10^{-1}$). The fluid–structure interaction simulation couples the discrete elastic rods algorithm with the method of regularized Stokes–let segments. Contact between two flagella is handled by a penalty-based method. We present a comparison between our experimental and simulation results and verify that the simulation tool can capture the essential physics of this problem. Preliminary findings on robustness to buckling provided by the bundling phenomenon and the efficiency of a multi-flagellated soft robot are compared with the single-flagellated counterparts. Observations were made on the coupling between geometry and elasticity, which manifests itself in the propulsion of the robot by nonlinear dependency on the rotational speed of the flagella.

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1 Introduction

Locomotion of micro-swimmers has drawn significant attention in biology and fluid dynamics since the 1950s.^{1–6} On a microscopic scale, the physics of the fluid is dominated by viscosity over the inertial effect. A seminal paper by Purcell in 1977 explains that reciprocal motions do not provide propulsive force for microswimmers.⁵ Instead, several natural microswimmers use the polymorphic transformation of multiple or single slender filamentary appendages (*e.g.*, cilia and flagella) to create nonreciprocal motion suitable for propulsion at low Reynolds number flow. Some cells, such as sperm and *Vibrio cholerae*, utilizes single cilium and flagellum to move under a low Reynolds number. In contrast, a metachronal wave of ciliary arrays in humans and mammals and multiple flagella of *Escherichia coli* exploits the interaction of multiple filamentary appendages with surrounding fluid for propulsion. Despite the differences in the number of appendages, many species of

bacteria utilize the elastic helical flagellum/flagella as the main geometric structure to interact with the low Reynolds number flow. However, the mechanism of multi-flagellated locomotion and single-flagellated is fundamentally different.

Multi-flagellated microswimmers have two modes of locomotion: “run” and “tumble”.^{2,7,8} Run is a period of near straight line motion caused by the flagella’s bundling. As multiple left-handed helix-shaped flagella turn in counterclockwise (CCW) direction for *E. coli*, the flagella turn and synchronize to form a single or multiple bundles of helical shape.⁹ On the other hand, a tumble is a period of random directional change caused by a change in the rotational direction of flagella, *i.e.*, if single or multiple flagella of *E. coli* rotates in clockwise (CW) direction. In essence, the multi-flagellated mechanism is an intricate interplay between geometric nonlinearity, hydrodynamics, and contact, contributing to robust bundling and direction-changing tumbling.

Inspired by the complexity of mechanics behind the simple driving mechanism, mechanical engineers also tried to formulate the motion of multi-flagellated bacteria.^{10–13} Only recently, the bundling behavior was shown to be purely mechanical due to the interaction of the soft helical structures and the viscous fluid.¹⁰ Further research on developing mechanical theory for flagellated locomotion beyond bundling and tumbling is also an active area of research. To fully understand the physics behind bacterial locomotion, the phenomenon such as synchronization

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and tangling of the bacterial flagella are being investigated.^{14–16} Besides its complexity in physics, the multi-flagellated mechanism is vital from both robotic and biological perspectives due to the following features: (1) directional stability,² (2) redundancy of actuation,¹⁷ (3) chemical secretion using flagella,^{18,19} (4) improved efficiency in the swarm and propagation.^{20,21}

Compared to the multi-flagellated mechanism, locomotion used by bacteria with a single flagellum lacks interaction with one or more flagella, exploiting a similar yet different mechanism. Monotrichous bacteria such as *Vibrio cholerae* exploit buckling instability induced by the hook of the flagellum to make a directional change in their motion.²² Consequently, numerous biological findings,^{2,7,8,23–26} mechanical experiments,^{10,27} hydrodynamic theories for low Reynolds flow,^{1,3,5,28,29} and medical microbots^{30–33} explored and exploited such a mechanism.

Despite the differences in the mechanism of locomotion, both multi-flagellated and single-flagellated locomotion are related in that it is a crucial fluid–structure interaction prevalent in the microscopic world. Prior works on soft robots actuated by flagella have considered simulation and experiments. To solve this fluid–structure interaction problem, the computational fluid dynamics model and slender body theory (SBT) were used to predict the motion of a single flagellated small-scale robot with rigid flagellum,^{34,35} ignoring the effect of flexibility of the flagella. With recent advancements in computational capability, the structural flexibility in a single-flagellated system can also be accounted for;^{36–38} the flagellum can be modeled as a linear elastic Kirchhoff rod.³⁹ Multiple studies have demonstrated the modeling of multi-flagellated systems.^{40–44} However, the coupling between long-range hydrodynamics, geometrically nonlinear deformation, and contact, has not been accounted for until recently.⁴⁵

In the field of microbots, several studies investigated the effect of multi-flagellated mechanisms. Due to the limited modes of locomotion that a single flagellated mechanism provide, Beyrand *et al.* presented multiple flagella microswimmers that can roll, run, and tumble.³¹ Ye *et al.* investigated multiple flagellated locomotion's benefits and the advantages of sinusoidal 2D geometry.³² Even bio-hybrid microbots have been developed, created by assembling biological flagellated organisms with the artificial magnetic structure, showing remarkable results of controlled locomotion using magnetic field.^{12,46} However, due to the nontrivial coupling between hydrodynamics, contact, and elasticity, researchers investigated lower-order coupling to solve the problem. *e.g.*, (1) using rigid flagellum for a flagellated robot under viscous fluid,^{34,35} (2) using a single elastic flagellum without modeling self-contact^{36,37} or (3) using ribbon-like multiple flagella without bundling behavior.^{31,32} A comprehensive numerical model and physical prototype for flagella bundling still need further investigation.

This paper presents a macroscopic soft robotic platform based on the propulsive mechanism of flagellated microorganisms and a physics-based computational framework to simulate the robot. The computational tool uses the Discrete Elastic Rods (DER) algorithm for elastic rod dynamics, Regularized Stokeslet Segments (RSS) method for hydrodynamics, including

long-range interaction,²⁹ and Spillman and Teschner's method of contact.⁴⁷ We first verify the simulation against the experiments with qualitative and quantitative comparisons. The simulation successfully captures the attraction between two flagella from hydrodynamic interaction. Following a quantitative comparison between experiments and simulations, the model's shortcomings are discussed, and directions for future research are suggested. We find from experiments and simulations that the flagella buckling⁴⁸ does not occur through purely hydrodynamic interactions between each flagellum for the multi-flagellated mechanism, while a single flagellated system may undergo buckling due to excessive hydrodynamic loads. Efficiency comparison between a single- and a multi-flagellated system shows that the single-flagellated robot has a slight efficiency advantage over its multi-flagellated counterpart. This simulation and the observations on the propulsive mechanism will set the foundation for further developing the soft robotic prototype. Furthermore, we report the experimental finding on cyclic unbundling without changing the velocity input.

2 Methods

2.1 Experimental setup

For experimental data collection, we used glycerin as the viscous medium for our robot. A cylindrical tank with a diameter of 28 cm and height of 45 cm was used with glycerin filled up to a height of approximately 40 cm. The robot was initially placed at the center of the glycerin tank to remain approximately 10 cm apart from the sidewalls, as depicted in Fig. 1. From the theoretical analysis based on Jawed and Reis,⁴⁹ and Liu *et al.*,⁵⁰ the distance of 10 cm from the wall minimally affects the propulsion of our prototype. The experimental footage and explanation on robot placement can be found on Supplementary methods section S1.A (ESI†). For every experiment, temperature and viscosity were measured. Viscosity was measured using USS-DVT4 rotary viscometer, and the viscosity measurement was in good agreement with the nominal value of the glycerin; dynamic viscosity of $\mu = 0.956 \pm 0.2$ Pa s. The temperature of glycerin was approximately 22 °C throughout the experiment to minimize the effect of temperature on viscosity. The fluid was mixed thoroughly before the experiment to avoid variation in density inside the tank.

The robot head contained Wemos D1 mini microcontroller unit used for the motor control, two 3.7 V 500 mA h lithium polymer (Lipo) batteries, and two mini geared DC motors. The motor was calibrated for angular velocity using Cybertech DT6236B Tachometer. Pulse width modulation (PWM) and rpm was calibrated within $\pm 1(0.01\%)$ rpm at 3.8 V. The head is in cylindrical shape with radius of 3.1 ± 0.01 cm and height ($h = 8.2 \pm 0.01$ cm) and was built using fused deposition modeling (FDM) 3D printer with polylactic acid plastic (PLA) material ($\rho = 1.26$ g cm^{−3}). The robot head was comprised of the casing and the main body. Urethane wax was applied inside the casing, outside the main body, and in the motor chamber to further prevent the glycerin from penetrating the robot. The

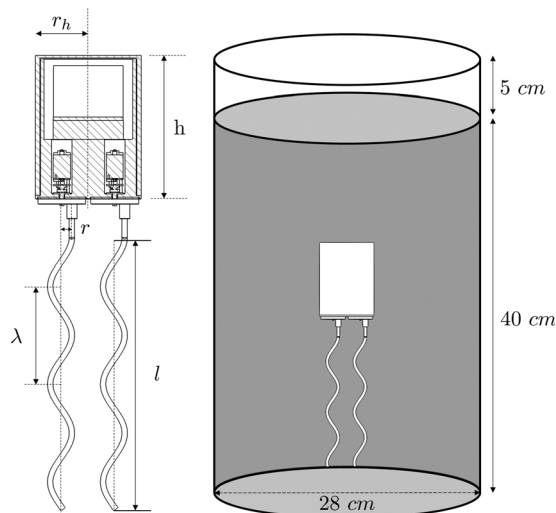


Fig. 1 Robot schematic, symbolic notations, and experimental setup. r_h denotes the radius of the robot head, and r denotes the radius of the helical flagellum. λ denotes the helix pitch, h denotes the height of the cylindrical head, and l denotes the axial length of a flagellum. The robot tank was filled with glycerine in a cylindrical tank with a diameter of 28 cm and filled to 40 cm.

ballast was placed near the robot centroid for neutral buoyancy. The design of the robot was intentionally bottom-heavy to ensure stability. Flagella were attached to the bottom plates that are connected to the motors.

For the flagella, Vinyl Polysiloxane (VPS) elastomeric material was used for fabrication with Young's modulus $E = 1255 \pm 49$ kPa and Poisson's ratio $\nu \approx 0.5$ (*i.e.* nearly incompressible). Catalyst and base – both liquid – were mixed with a 1 : 1 volume ratio. Iron fillings were added to the liquid mixture to match the density of the glycerin ($\rho = 1.26 \text{ g cm}^{-3}$). Left-handed helix shaped molds with different pitch parameters ($\lambda = 3.18, 4.45, 5.72$ cm) were 3D printed. Hollow polyvinyl chloride (PVC) tubes were placed inside the molds, and the liquid mixture was injected inside the tubes. After waiting a few hours to cure, the PVC tubes were cut out, and filamentary soft helical rods were obtained.⁵¹ More information on the choice of the geometry for both head and artificial flagella are available on Supplementary methods section S1.B (ESI[†]).

The robot was activated from 30 rpm to 70 rpm at 10 rpm intervals. The corresponding Reynolds number for the flagella ($\text{Re} = \frac{\rho \|\omega_T \times r\| r_0}{\mu}$), ranges from 0.0232–0.0943. the video of the robot submerged inside the glycerin tank for over 300 seconds for each rotational speed was recorded for data collection. Out of the 300 seconds, we used the data between 30 and 270 seconds to ignore the initial transience during the speed ramp-up from 0 rpm to a prescribed total rpm, which is the sum of ω_t and ω_h depicted in Fig. 2. Then, the videos were converted into jpg files with a frame rate of 1 frame per second. The image files were then processed using stacked image processing centroid calculation using the ImageJ image processing tool.

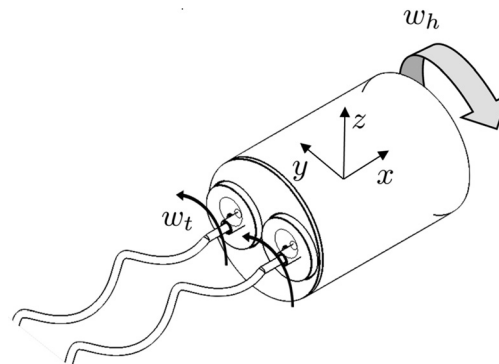


Fig. 2 Schematics of the robot. Rotational motions are exclusively denoted to show that both rotation of the head and rotation of the tail occurs. The body-fixed frame is shown in the center of the flagella robot to define the direction of rotation. The head rotates with angular velocity ω_h around the x -axis of the body-fixed frame, and tail rotates with angular velocity ω_t around the center of each helix.

2.2 Physics-based simulation of the soft robot

Fig. 3 shows the discretized schematic of our robot. The rod is discretized into N nodes: $\mathbf{x}_k = [x_k, y_k, z_k]^T$ for $0 \leq k \leq N - 1$, and $N - 1$ corresponding edges: $\mathbf{e}^k = \mathbf{x}_{k+1} - \mathbf{x}_k$ for $0 \leq k \leq N - 2$. The degree of freedom (DOF) vector of discretized robot is defined as $\mathbf{q} = [\mathbf{x}_0^T, \theta^0, \mathbf{x}_1^T, \theta^1, \dots, \mathbf{x}_{N-2}^T, \theta^{N-2}, \mathbf{x}_{N-1}^T]^T$, where θ^k is the scalar twist angle at edge $\mathbf{e}^k$. Therefore, the size of the DOF vector for N nodes is $4N - 1$. Hereafter, subscripts are used for the node-based quantities, and superscripts are used for the edge-based quantities.

An important characteristic of the DER method is the computation of the twisting of a rod simply by using a set of single scalar quantities θ^k embedded in the DOF vector. In this formulation, each edge has a reference frame (noted as $\mathbf{d}_1^k, \mathbf{d}_2^k, \mathbf{t}^k$ in Fig. 3) that is orthonormal and adapted (*i.e.* $\mathbf{t}^k$ is the tangent

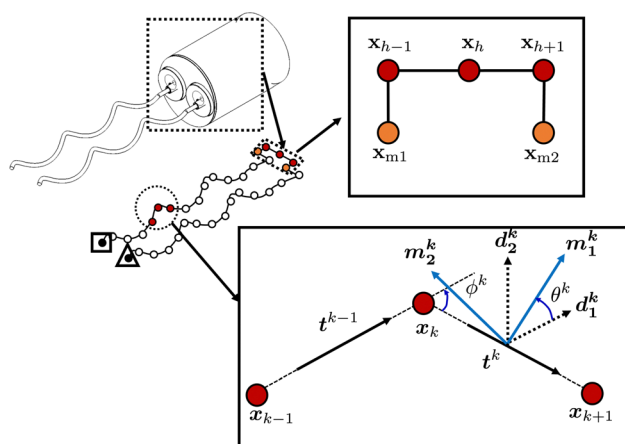


Fig. 3 Schematic showing discretization of the soft robot. The robot is modeled as a single rod starting from the left end of the flagella (denoted as a square) and ending at the right end of the flagella (denoted as a triangle). The head is modeled using three nodes (denoted as red dots). The center of the head is $\mathbf{x}_h$. The nodes to the left and right of the center are $\mathbf{x}_{h-1}$ and $\mathbf{x}_{h+1}$, respectively. Two orange dots, $\mathbf{x}_{m1}$ and $\mathbf{x}_{m2}$, are the nodes where the flagella are actuated.

along the k th edge). The construction of the reference frame is first initialized at the first edge ($k = 0$) at time $t = 0$ with an arbitrary set of orthonormal vectors (with the condition that the third vector $\mathbf{t}^0$ is the tangent to the first edge). Then, the reference frame is parallel transported⁵² to the subsequent edges to form the reference frame on all the edges. After this initialization, the reference frame can be updated at each time step by parallel transporting $\mathbf{d}_1^k, \mathbf{d}_2^k, \mathbf{t}^k$ from the “old” configuration (DOF vector before the time step) to the “new” configuration (DOF vector after the time step). The material frame is also an adapted orthonormal frame (noted as $\mathbf{m}_1^k, \mathbf{m}_2^k, \mathbf{t}^k$ in Fig. 3) that is identical to the reference frame at $t = 0$. Since both the frames share a common director ($\mathbf{t}^k$), a single scalar quantity – the twist angle, θ^k – can be used to compute the material frame from the reference frame. An algorithmic representation of this update of the frame is shown in Algorithm 1.

Based on the discretization, the elastic strains are required to calculate the energy and formulate the equations of motion (EOM) to march from time $t = t_i$ to time $t = t_{i+1} = t_i + \Delta t$, where Δt is the time step size in the simulation outlined in Algorithm 2. An elastic rod has three types of strains – bending, twisting, and stretching – associated with its deformation. We use the physical parameter presented in Table 1 for the calculation of the strains. Using these strains, we can calculate our system's stretching, bending, and twisting energy; the sum of three energy is noted as the elastic energy and is represented as Eqn (1). Details on the calculation of the strains and energy term can be found on Supplementary methods section S2 (ESI†).

$$E_{\text{elastic}} = \underbrace{\sum_{k=0}^{N-2} E_k^s}_{\text{stretching energy}} + \underbrace{\sum_{k=1}^{N-2} E_k^b}_{\text{bending energy}} + \underbrace{\sum_{k=1}^{N-2} E_k^t}_{\text{twisting energy}}, \quad (1)$$

We can simply take the gradient of the energy terms with respect to the DOFs to get the elastic force at each DOF. The elastic force at the k -th DOF is $-\frac{\partial E_{\text{elastic}}}{\partial \mathbf{q}_k}$. The simulation marches forward in time by updating the configuration, *i.e.*, DOF vector, of the robot based on EOM. We can even impart

artificial configuration updates in the simulation that are dynamic. In particular, for actuation of the robot we implement a time-dependent fixed-rate natural twist on nodes $\mathbf{x}_{m1}$, and $\mathbf{x}_{m2}$ shown in Fig. 3. To propagate in time, the equation of motion to be solved at the k -th node is

$$\mathbf{f}_k \equiv \frac{m_k}{\Delta t} \left[\frac{\mathbf{q}_k(t_{i+1}) - \mathbf{q}_k(t_i)}{\Delta t} - \dot{\mathbf{q}}_k(t_i) \right] + \frac{\partial E_{\text{elastic}}}{\partial \mathbf{q}_k} - \mathbf{f}_k^{\text{ext}} = 0, \quad (2)$$

where $\mathbf{q}_k(t_i)$ is the old position (and the k -th element of the vector $\mathbf{q}(t_i)$), $\dot{\mathbf{q}}_k(t_i)$ is the old velocity, m_k is the lumped mass at the k -th DOF, and $\mathbf{f}_k^{\text{ext}}$ is the external force on the k -th DOF. Note that eqn (2) is simply a statement of Newton's second law. External forces may include gravity, contact, and hydrodynamics, and the $(4N - 1)$ -sized external force vector can be written as

$$\mathbf{f}^{\text{ext}} = \mathbf{f}^{\text{h}} + \mathbf{f}^{\text{head}} + \mathbf{f}^{\text{c}}, \quad (3)$$

where $\mathbf{f}^{\text{h}}$ is the hydrodynamic force vector on the flagella, $\mathbf{f}^{\text{head}}$ is the hydrodynamic force vector on the head, and $\mathbf{f}^{\text{c}}$ is the contact force vector (Supplementary methods section S3, ESI†).

Now that the EOM is defined, we need to solve the system of $(4N - 1)$ equations defined by eqn (2) to compute the new position vector, $\mathbf{q}(t_{i+1})$. The Newton–Raphson method can be used to solve the equations which require the Jacobian of eqn (2). The (k, m) -th element of the square Jacobian matrix is

$$\mathbb{J}_{km} = \frac{\partial \mathbf{f}_k}{\partial \mathbf{q}_m} = \mathbb{J}_{km}^{\text{inertia}} + \mathbb{J}_{km}^{\text{elastic}} + \mathbb{J}_{km}^{\text{ext}}, \quad (4)$$

The expressions for the Jacobian terms associated with the elastic forces are available in the literature.⁵² The Jacobian terms associated with some external forces ($\mathbf{f}^{\text{h}}, \mathbf{f}^{\text{head}}$) cannot be analytically evaluated and those terms are simply set to zero. In other words, those forces are incorporated into the simulation in an Euler-forward fashion.

Algorithm 1 Multiflagella soft robot simulation

Require: $q(t_j), \dot{q}(t_j)$
Require: $(d_1^k(t_j), d_2^k(t_j), t^k(t_j))$
Ensure: $q(t_{j+1}), \dot{q}(t_{j+1})$
Ensure: $(d_1^k(t_{j+1}), d_2^k(t_{j+1}), t^k(t_{j+1}))$
1: Guess: $q^{(1)}(t_{j+1}) \leftarrow q(t_j)$
2: $n \leftarrow 1$
3: Calculate $\mathbf{f}^{\text{h}}$ and $\mathbf{f}^{\text{head}}$
4: ▷ **Supp. methods – Section S3 (ESI†)**
5: solved $\leftarrow 0$
6: **while** solved = 0 **do**
7: **while** error > tolerance **do**
8: Compute ref. frame using $q(n)$ ($t_j + 1$)
9: $(d_1^k(t_{j+1}), d_2^k(t_{j+1}), t^k(t_{j+1}))^{(n)}$
10: Compute ref. twist $\Delta m_{k,\text{ref}}^{(n)}$
11: Compute material frame
12: $(m_1^k(t_{j+1}), m_2^k(t_{j+1}), t^k(t_{j+1}))^{(n)}$
13: Compute $\mathbf{f}$ and $\mathbb{J}$ ▷ Eqn. (2) and (4)
14: $\Delta q \leftarrow \mathbb{J} \backslash \mathbf{f}$

Table 1 Table of geometric, physical, and simulation parameters with symbol representations

Parameter	Value (Exp/Sim)	Description
r	0.0064	Radius of helix (m)
λ	0.0572	Pitch of helix (m)
l	0.0954	Axial length of helix (m)
r_h	0.031	Radius of robot head (m)
r_0	0.0016	Radius of the rod (m)
E	1.255×10^6	Young's modulus (Pa)
ν	0.5	Poisson's ratio
ρ	1260	Density (kg m^{-3})
μ	$0.956 \pm 0.2/1.0$	Viscosity (Pa s)
Δt	1.0×10^{-4}	Time step
ε	1.67×10^{-4}	Regularization parameter
$ e $	5.0×10^{-3}	Discretization length (m)
C_t	4.8	Translational drag coefficient
C_r	0.36	Rotational drag coefficient

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15.    $q^{(n+1)} \leftarrow q^{(n)} - \Delta q$ 
16.   error  $\leftarrow$  sum (abs (f))
17.    $n \leftarrow n + 1$ 
18: end while
19: solved  $\leftarrow$  1
20: for  $l = 0$  to  $l = N - 2$  do
21:   for  $m = 0$  to  $m = N - 2$  do
22:     Compute  $\delta_{(l,m)}^{\min}$ 
23:     if  $\delta_{(l,m)}^{\min} < 2r_0$  then
24:       Compute  $\mathbf{f}_l^c, \mathbf{f}_{l+1}^c, \mathbf{f}_m^c, \mathbf{f}_{m+1}^c$ 
25:        $\triangleright$ Supp. methods – Section S4 (ESI†)
26:       solved  $\leftarrow$  0
27:     end if
28:   end for
29: end for
30: end while
31:  $q(t_{j+1}) \leftarrow q^{(n)}(t_{j+1})$ 
32:  $\dot{q}(t_{j+1}) \leftarrow \frac{q(t_{j+1}) - q(t_j)}{\Delta t}$ 
33:  $(d_1^k(t_{j+1}), d_2^k(t_{j+1}), t^k(t_{j+1})) \leftarrow (d_1^k(t_{j+1}), d_2^k(t_{j+1}), t^k(t_{j+1}))^{(n)}$ 

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After solving eqn (2) to calculate the new position $\mathbf{q}_k(t_{i+1})$, new velocity can be trivially computed from $\dot{\mathbf{q}}_k(t_{i+1}) = (\mathbf{q}_k(t_{i+1}) - \mathbf{q}_k(t_i))/\Delta t$.

3 Results and discussion

3.1 Validation of physics-based simulation of multi-flagellated robot

To demonstrate our simulation model's validity, we compared our multi-flagellated robot's locomotion against the simulation. For generality, we present our results in a nondimensional form. Due to the slender geometry of the system, bending is the dominant deformation mode. Balancing the elastic bending force and the external viscous loading yields a characteristic time scale of $\mu l^4/(EI)^{48,53}$. This characteristic time is used to nondimensionalize the time, and a characteristic bending force of EI/l^2 is used to nondimensionalize the forces. The distance was nondimensionalized with the axial length. Hereafter, overbar (—) represents normalized quantities, *i.e.* $\bar{t} = \frac{tEI}{\mu l^4}$,

$$\bar{\omega} = \frac{\omega \mu l^4}{EI}, \bar{v} = \frac{v \mu l^3}{EI}, \bar{F}_p = \frac{F_p l^2}{EI}, \bar{x} = \frac{x}{l}, \bar{\lambda} = \frac{\lambda}{r}, \text{ etc.}$$

Fig. 4a shows snapshots from experiments and simulations at three different values of pitch: $\bar{\lambda} = \{5, 7, 9\}$. From Fig. 4a, we first qualitatively analyze the match between the transitional motion of the flagella crossing and bundling behavior. We noted during experimental observations that the $\bar{\lambda} = 5$ case formed a bundle throughout the entire range of angular velocity variation (30 to 70 rpm). On the other hand, $\bar{\lambda} = 7$ case formed a partial bundle at 50 and 60 rpm, and $\bar{\lambda} = 9$ did not bundle but had continuous contact between two flagella. In Fig. 4b, we present quantitative comparison of experimental

data with simulation at 30, 40, and 50 rpm for $\bar{\lambda} = 7$ and plot the position of the robot along x and y directions against normalized time. The data frequency of the experiment is one frame per second (fps), and the data frequency of the simulation is ten fps.

We obtain the values of the numerical prefactors C_t and C_r by data fitting using data obtained on experiment with $\bar{\lambda} = 7$. Details on the numerical prefactors are found on Supplementary methods section S3 (ESI[†]). By comparing the mean total least squared error for the axial velocity v , rotational velocity, the prefactors that provided minimal error between the experiment and simulation were used. Both prefactors are the coefficients to account for the non-spherical shape of the robot body in translational, rotational hydrodynamic drag calculation based on the sphere at Stokes flow.

The experiment and simulation results show reasonable agreement in the positional data for $\bar{x}$ and $\bar{y}$ in Fig. 4b. The normalized x position, $\bar{x}$, shows a better match between the simulation and experiment (Fig. 4b.1). The normalized y position, although the experiment follows similar oscillatory trend, the experimental robot exhibited smaller average magnitude with higher standard deviation. From Fig. 4b.2, we can observe that as the angular velocity increases, the oscillation frequency in normalized y position increases accordingly. This represents an undulatory sideways motion of the robot as it moves upward (along x direction). Even though both experiments and simulations show the same trend, there exist discrepancies in the higher rpm and lower normalized pitch cases. We attribute this to the friction between the flagella surfaces. Unlike simulation, where we resolve contact between the two flagella without consideration of friction between each flagellum, we observed in our experiment that once it partially or fully bundles, the bundled part has a high frictional force that makes the flagella be kept in the bundled configuration when transitioning to the partially bundled regime. Simple moment balance tells us that the cell body (*i.e.*, the head of the robot) and the flagella have to rotate in opposite directions for net zero torque. It is known through previous works that the counter-rotation of the cell body in bacterial locomotion contributes to the trajectory and efficiency of the organism and could even contribute to the bundling of the flagella.^{54,55} We use our robot to investigate the rotation of the head and, in Fig. 5, plot the angular velocity of the head as a function of the total angular velocity from both experiments and simulations at three different values of the pitch. The error bar is obtained from the standard deviation of the experimental values. At lower values of total angular velocity ($\bar{\omega}_T \lesssim 100$), there is little variation in the angular velocity of the head at different pitch values. In both experiments and simulations, we see that the angular velocity of the head increases almost linearly with the total angular velocity. We exploit our simulations to probe the higher angular velocity regime and clearly see that the head angular velocity increases sublinearly with the total angular velocity. The variation in the head angular velocity as a function of the pitch of the flagella is worth mentioning. Among the three examined here ($\bar{\lambda} = \{5, 7, 9\}$), the head angular velocity is the highest at $\bar{\lambda} = 7$. This nonlinear

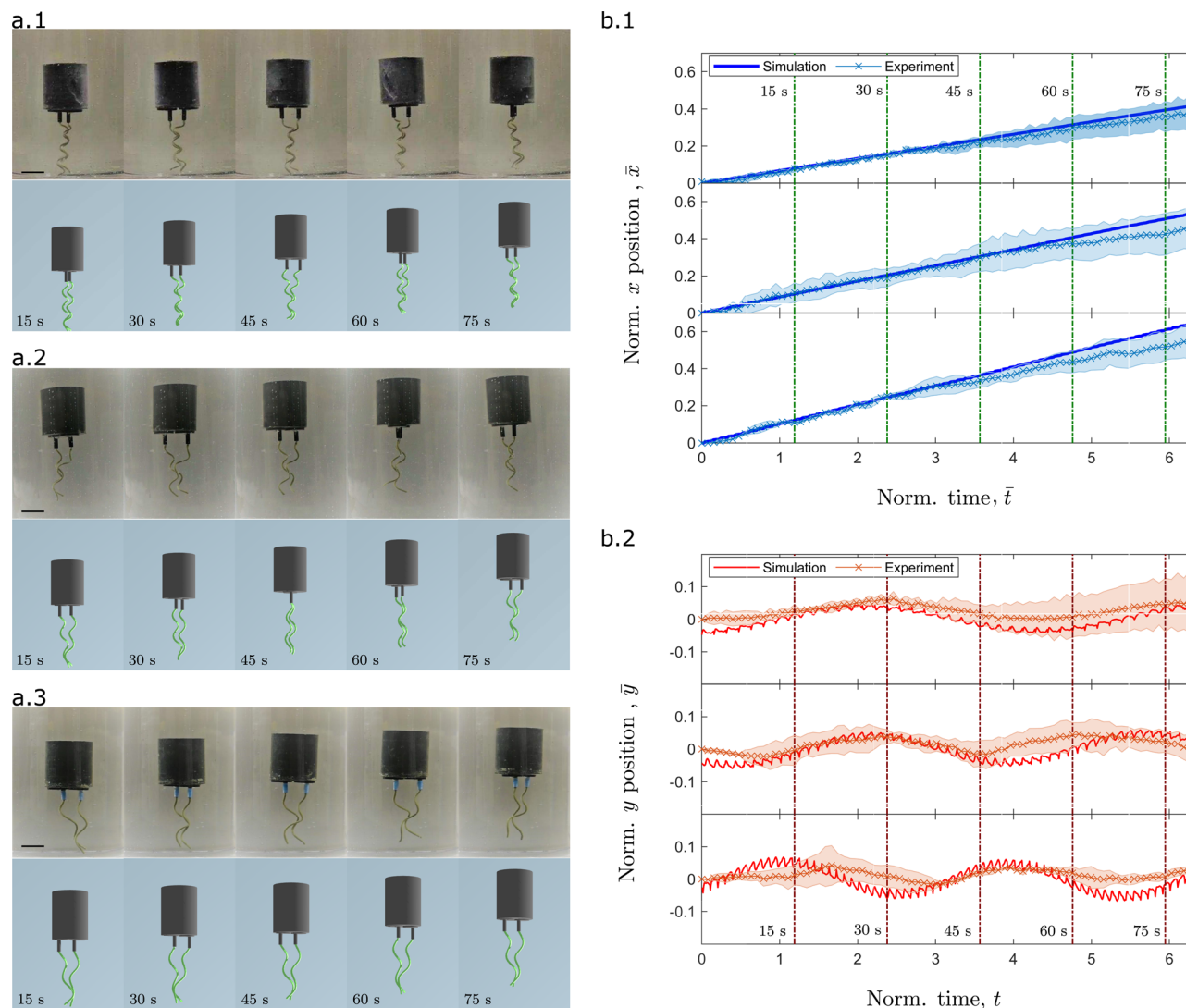


Fig. 4 Comparison of data for experiment and simulation for different pitch to helix radius ratio of flagella ($\bar{\lambda} = 5, 7, 9$): (a) snapshot comparison between experiment and simulation at 60 rpm, scale bar: 3 cm. The deformation of elastic filamentary flagella in experiment and simulation has a plausible agreement; (b) comparison of experimental data with simulation at 30, 40, 50 rpm for $\bar{\lambda} = 7$. (b.1) compares normalized x position, and (b.2) compares normalized y position against normalized time. The shaded area represents the standard error of experiment data. Normalized time for the snapshot in Fig. 5 (a) is drawn as dotted lines with time notations in Fig. 5 (b).

dependence on the flagella's geometric parameter (pitch) may be counterintuitive; however, it is a manifestation of the problem's highly nonlinear and coupled nature. This type of nonlinearity with a variation of geometry for a rigid helical structure can also be found in ref. 27, which used a single-flagellated system and analyzed the normalized force with respect to the normalized pitch. However, from our experiment and simulation, we observed that the coupling of the elasticity results in a different nonlinear pattern in the velocity of the robot, which is relevant to the forces in the direction of propulsion from the previous work done with a rigid structure. This result shows a new outlook for future research to determine the relationship between the elasticity, bundling, and hydrodynamic effect that changes previously known geometric

dependency on the force and torque for a single rigid helical structure.

Next, in Fig. 6, the velocity of the bacteria robot along the x-axis is shown as a function of the normalized total angular velocity, $\bar{\omega}_T$. The error bar represents the standard deviation of the normalized x-velocity. The x-velocities are obtained through the coefficient of the linear fitting of the position value through MATLAB polyfit function. Interestingly, the translational velocity increases superlinearly with the total angular velocity in the regime explored here. The nonlinear dependence of translational velocity on the pitch of the flagella is also apparent. The case with $\lambda = 7$ results in lower propulsive speed than the $\lambda = 5$ and $\lambda = 9$ cases. In Fig. 6, the simulation results overestimate the velocity of the experimental robot.

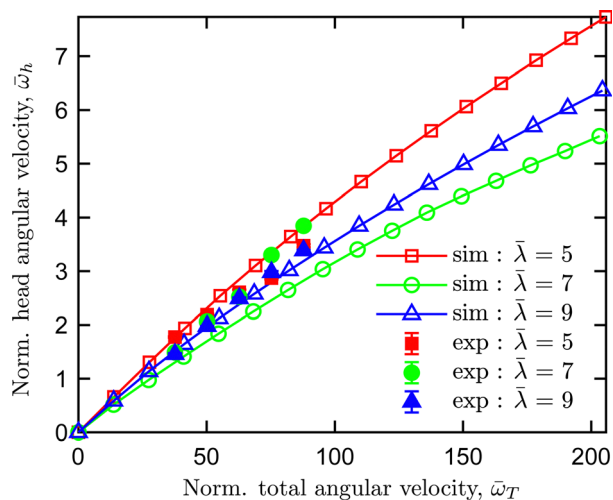


Fig. 5 Comparison of simulation and experiment for head and total angular velocity. The experimental data are in symbols with error bars.

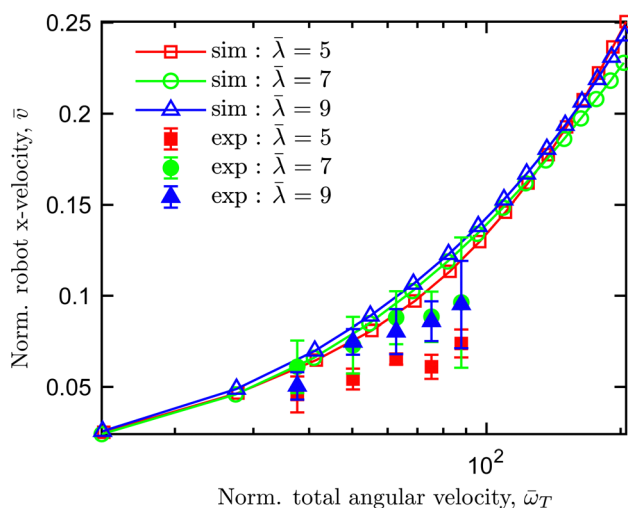


Fig. 6 Nonlinear relationship of angular velocity and robot x-velocity captured through simulation. The experimental data are in symbols with error bars.

This discrepancy in simulation and experiment can be attributed to the friction between the two flagella that was observed in experiments. Since the amount of contact is more dominant at lower pitch values, the experiments and the simulations differ further for the case with $\bar{\lambda} = 5$ compared with $\bar{\lambda} = 7$ and $\bar{\lambda} = 9$ cases. At this stage of our research, the simulation tool enforces non-penetration conditions but does not incorporate friction. This implies that one flagellum can smoothly slide past another flagellum without any resistance from friction. However, that is not the case in the real world. In experiments, the flagella form a tighter bundle compared with simulations, leading to a lower net propulsive force forward. Incorporating physically-accurate friction inside a low Reynolds environment is a direction of future research. The simulation tool presented in this paper, which models the entire system as a single rod for computational

efficiency, can be used to explore various models of friction and eventually formulate an accurate model that matches experiments. A few recent works have explored friction among rods in simpler settings,^{56,57} and our simulations can be augmented to include such friction models.

3.2 Comparison with single-flagellated robot

In this section, we take one step toward a mechanistic understanding of the difference between these two modes of locomotion – single-flagellated and multi-flagellated. Locomotion of a robot (or bacterium) with a single flagellum was recently investigated using a DER-based numerical framework.³⁷ A single-flagellated robot cannot exhibit bundling; however, it can undergo buckling instability beyond a critical value of the total angular velocity when the resulting external hydrodynamic force is too large. In Fig. 7, we utilize our same simulation tool to model a single-flagellated robot.

We assumed that all the parameters were the same between the single-flagellated robot and the multi-flagellated case discussed above. The only difference is the number of flagella. Fig. 7a shows the Euclidean distance, L' , between the head node and the tail node (the node at the free tip of the flagellum) as a function of the total angular velocity, ω_T , obtained from simulations. This apparent length, L' , has been normalized by its value at $\omega_T = 0$ so that all the curves for three different pitch values start at (0,1). The star symbols represent the angular velocity beyond which the apparent length, L' , of the robot abruptly drops, and the flagellum buckles. Two snapshots – one of an unbuckled configuration and one of a buckled shape – are also shown in Fig. 7a. For $\bar{\lambda} = 5$, the flagella buckles at $\bar{\omega}_T \approx 230$ and the $\bar{\lambda} = 7$ case buckles at $\bar{\omega}_T \approx 363$. The case for $\bar{\lambda} = 9$ does not buckle in the regime explored in this figure. The findings on the single-flagellated robot are similar to the study in Huang *et al.*³⁷

Next, we employ the simulation tool to comparatively explore the propulsive forces of the two types of systems – single-flagellated and multi-flagellated. Fig. 7b shows the non-dimensionalized propulsive force as a function of total angular velocity at three different pitch values for both the single-flagellated and multi-flagellated cases. Propulsive force is defined as the x-component (direction of motion of the robot) of the force exerted on the head (eqn (S15), Supplementary methods section S3, ESI†). The propulsive force for the multi-flagellated robot was divided by the number of flagella. The propulsive force generated by the robot is small (on the order of 10^{-3} N), which makes it difficult to measure experimentally. Our robotic platform does not have a force sensor; therefore, we use simulations to analyze the propulsive force and efficiency of the soft robot. The trend is qualitatively different between the two cases. For single-flagellated robot buckles at a critical angular velocity (indicated by star symbols), and its propulsive force dramatically drops at that point. The multi-flagellated robot does not exhibit buckling behavior even at larger angular velocities; the flagella bundle instead. Even though the computational simulation cannot accurately account for the physical friction, Fig. 7b shows that buckling for multi-flagellated mechanism

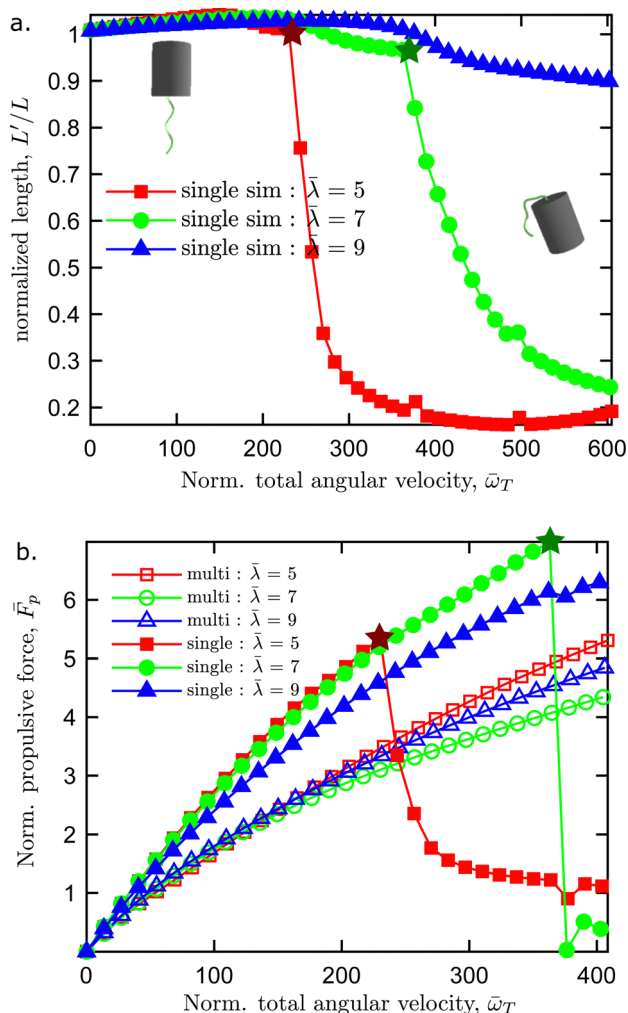


Fig. 7 Comparison between single-flagellated robot and multi-flagellated robot simulation: (a) plot of a normalized tail to head distance with respect to the normalized angular velocity. Star symbols represent the critical angular velocity where the flagellum buckles. Rendered image of unbuckled (left) and buckled (right) state of the robot shown within the graph. (b) A figure of normalized propulsive force with respect to the normalized angular velocity. Star symbols represent the buckling.

is not purely hydrodynamic interactions unlike the single flagellated mechanism.⁴¹ A point of note is the relatively larger propulsive force per flagellum in the single-flagellated robot prior to buckling than in the multi-flagellated robot. The propulsive force depends on the deformed shape of the flagella, and this shape differs between the single-flagellated case (no bundling, only buckling) and the multi-flagellated case (prominent bundling). However, the propulsive force is larger in the multi-flagellated system beyond the critical threshold for buckling in a single-flagellated robot. In short, a single-flagellated robot generates a larger propulsive force per flagellum; however, its propulsion is limited by instability. The non-monotonic dependence of propulsion force on the geometry of the flagella (pitch) is observed in the multi-flagellated case. The robot with $\bar{\lambda} = 5$ generates the largest force and $\bar{\lambda} = 7$ generates the least; $\bar{\lambda} = 9$ falls in between. In contrast, a single-flagellated robot generates more propulsion as

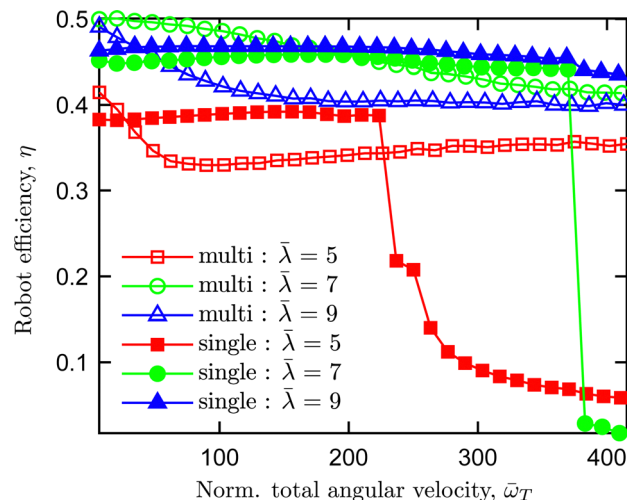


Fig. 8 Efficiency graph for the single and multi flagella robot simulation. Efficiency is defined as the ratio of the force and torque of the head. Due to flagella interaction, the multi-flagellated robot has lower efficiency.

the pitch decreases. However, this observation is true only for the range of parameters explored in this study. Prior works²⁷ show non-monotonic dependence of propulsion on the pitch of the flagellum; however, the flagellum was assumed to be rigid.

The observations on propulsive force lead us to address the efficiency of the flagellated robots using numerical simulations. Fig. 8 shows the variation of efficiency with the total angular velocity at three pitch values in both cases. Efficiency is defined as $\eta = \frac{f_h^{\text{head}} \cdot r_h}{T_h}$, where f_h^{head} is the hydrodynamic force on the head, and T_h is the torque due to rotation of the head. Qualitatively, efficiency is a measure of the ratio of the propulsive force and the torque exerted by the motor. At smaller values of angular velocity, multi-flagellated robot decreases in efficiency. This decrease is particularly prominent at small pitch values and, thus, high interaction between flagella. Efficiency is the highest when $\bar{\lambda} = 7$ and lowest at $\bar{\lambda} = 5$, which further signifies the nonlinear nature of the problem. If the robot has a single flagellum, there is no bundling, and the shape of the flagellum remains almost helical until the threshold for buckling. Therefore, the efficiency remains almost constant as a function of angular velocity before buckling. The efficiency drops to almost zero post-buckling.

3.3 Bundling and unbundling sequence

In this section, we report the observed sequence of bundling and unbundling found in the experiment. As stated in Section 3.1, bundling was most exhibited at: (1) higher rotational velocity, (2) lower pitch value. While bundling behavior is captured in both simulation and experiment, unbundling was only captured in the experiment. Previous research on unbundling that does not involve a directional change in the rotation of one or more flagella is limited. Reigh *et al.* found a stable bundled region characterized by flagella anchor distance and applied torque differences for a multi-flagellated system. The

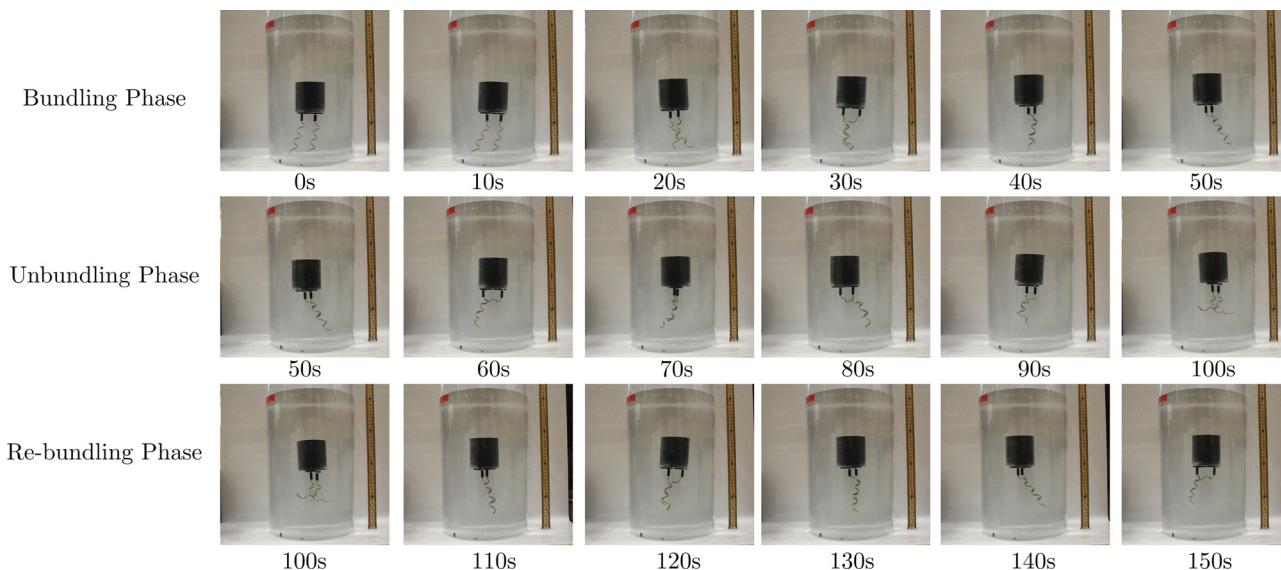


Fig. 9 Periodic bundling, unbundling, and re-bundling phase. The snapshot is for the case where $\bar{\lambda} = 5$ at 50 rpm. Without any change in the rotational velocity input, and due to the contact-initiated friction and slippage, the unbundling occurs. Leading to cyclical behavior of bundle and unbundle of flagella, which was not captured in the simulation.

authors of the paper show simulation results on how slippage affects the unbundling process and suggests that slippage may lead to tumbling behavior of bacterial locomotion.⁵⁸

In Fig. 9, the robot at 50 rpm with $\bar{\lambda} = 5$ exhibits bundle and unbundle phase. This cyclical behavior was shown throughout at 40–70 rpm for the case with $\bar{\lambda} = 5$. As expected, the initial bundling, while going through the transient phase, occurs for an extended period (50 s) than the re-bundling phase to get back to a fully bundled state (10 s). After both flagella fully bundle, the unbundling starts. The unbundling process is shown as one of the flagella starting to slip along the bundled helix. After approximately 50 s, the bundle reaches a fully unbundled shape. Snapshot at 50–90 s and 110–150 s on Fig. 9 displays that the unbundling phase repeats in the same geometric manner after the full bundle occurs. We suspect the reason for this to be the friction between the two flagella and a possible mismatch in torque due to experimental limitations. After the bundle has been formed, the bundle starts to skew as the contact friction increases. One flagellum tries to get out of the bundle while the friction tries to hold the bundle. As one flagellum slowly escapes from the bundle, the part with friction holds the flagellum that tries to escape from the bundle. However, the unbundled part starts pumping the remaining flagellum out by repeated buckling of the escaping flagellum's unbundled region.

4 Conclusion

In conclusion, we presented a multi-flagellated soft robotic platform and a numerical simulation method. These tools were used to explore the relationship between the motion of the robot and the geometry of the flagella. Both the experiments

and simulations could capture the bundling behavior of the elastic flagella caused by long-range hydrodynamic interaction. Bundling is only possible if the flagella are flexible and there is long-range interaction by flows induced by distant parts of the flagella. Prior works often neglected the flexibility of the flagella or ignored the long-range hydrodynamics in favor of a simplified (but computationally cheap) resistive force theory-based hydrodynamic model.¹ Our study emphasizes the need to accurately capture these two ingredients – flexibility and long-range hydrodynamics – in modeling bacteria and robots inspired by them. The simulation tool can successfully capture both elements.

The accuracy of the simulation, when compared to the experiment, was reasonable, where our metrics for comparison were the translational velocity of the robot and the angular velocity of the head. The lack of an accurate friction model was identified as the main reason behind any mismatch between experiments and simulations and a potential contributing factor to unbundling, which simulation could not capture. This simulation and the experimental platform provide a basis for the future development of multiple flagella-based robots. The results were presented in a nondimensional format. As long as the dimensionless groups are the same (*e.g.*, Reynolds number is low), they apply to robots and organisms of any size.

The robotic platform can be easily re-purposed to explore tumbling – change in the direction of swimming – when one flagellum rotates in a direction opposite to the other flagellum. In addition, the robot can be improved by integrating sensors and an inertial measurement unit (IMU) to achieve 3D trajectory control of the robot.

Directions for future work include (1) analysis of the tumbling and unbundling behavior, (2) incorporation of a physically accurate friction model, (3) investigation of the role of

head flexibility and geometry, (4) formulation of control policy along with hardware improvement for an autonomous robot. Despite these limitations, we are close to realizing palm-sized flagellated robots that are simple in design (few moving parts) and control (angular velocity is the only control input) yet functional (*i.e.*, capable of following 3D trajectory by bundling and tumbling). With the ongoing advancements in biological discoveries, mechanical experiments, theories, and simulation, we envision that our research can lead to a small, simple, cheap, but functional robot that could fully capture the locomotion of bacteria.

Conflicts of interest

The authors declare that they have no conflict of interest.

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