Improved Kinematic Models for Two-Link Helical Micro/Nanoswimmers

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Abstract—Accurate prediction of the 3-D trajectories of micro/nanoswimmers is a key element to achieve high precision motion control in therapeutic applications. Rigid-body kinematics of such robotic systems is dominated by viscous forces. The induced flow field around a two-link swimmer is investigated with a validated computational fluid dynamics model. Force-free-swimming constraints are employed in order to simulate motion of bacteria-like swimmers in viscous medium. The fluid resistance exerted on the body of the swimmer is quantified by an improved resistance matrix, which is embedded in a validated resistive force theory model, based on a complex-impedance approach. Parametric studies confirmed that the hydrodynamic interaction between body and tail are of great importance in predicting the trajectories for such systems.

Index Terms—Biological cells, biomechatronics, fluidic microsystems, hydrodynamics, numerical models, robot kinematics, velocity measurement.

I. INTRODUCTION

SWIMMING micro- and nanorobots in the literature are presented as the candidates of minimal-invasive surgery tools to handle high precision therapeutic operations such as retina repair [1], [2]. Based on observations on bacteria and spermatozoa, and via some macro and microscale experiments, propulsion mechanisms of natural microswimmers are established as viable actuation means for motile autonomous swimming microrobots [3]–[10]. Propulsion mechanisms of bacteria and spermatozoa are based on wave propagation carried out by slender tail structures that are actuated by nanoscale motors [11]. The motivation of this study is to identify the role of hydrodynamic interactions (HI) between body and tail on the effective drag force and rigid-body kinematics of bacteria species, and to present modeling tools that improve the predictability of swimming trajectories of bacteria, which are to be incorporated in cybernetic micro/nanorobotic systems as the means of propulsion and navigation solving key problems such as energy supply to artificial bioinspired swimmers. In that regard, E. Coli species are considered ideal examples of nanoscale devices [12].

A. Literature Review

Experimental work is carried out to manufacture rotary motors in microdimensions [13]; however, the size and complexity of the bacterial motor [14] are the bottlenecks in construction of a working replica, which compel researchers to execute artificial means of actuation [4], [8], [9] in order to achieve untethered bioinspired microswimming.

In order to mimic natural swimmers, different actuation mechanisms are employed: generating planar waves driven by external magnetic fields on an artificial magnetic tail attached to a red blood cell [4], employing dedicated dc motors to rotate helical tails in order to control the motion of the bioinspired robot [8], or rotating the magnetic body of single-link helical swimmers with magnetic fields driven by Helmholtz coils in order to generate screw-like motion in viscous fluids [9], [10]. However, the energy efficiency of such artificial systems is actually lower than that of the bacterial motor [15].

As another strategy, some bacteria species are considered the controllable means of actuation or propulsion for a variety of microsystems provided that given proper conditions and incentives they already possess the capability of maneuvering themselves [16]. One likely use for cybernetic microsystems is carrying out therapeutic operations in living tissue; by means of either controlling a single bacterium as a nanorobot or using the bacterium cell as an integral part in microfluidic microsystems for transport and actuation purposes [17], [18].

The possibility of moving objects via natural swimmers that employ a bacterial motor is experimentally studied with groups of S. Marcescens specimens attached to a cargo [19]. The authors investigated the propulsive forces, towing velocity and adherence durability in time. Martel [20] studied controlling the swimming direction of a magnetotactic bacteria (MTB) species, i.e., M. Gryphiswaldense, by inducing external magnetic fields, which in turn incorporates bacterial swimming with computer control. It is observed that the selected specimens follow the induced magnetic field lines. Martel et al. [21] manipulated single beads of 3 μm as cargo by controlling the velocity of individual MTBs. They further reported that reaching velocities faster than 100 μm/s in magnitude is achievable [21]. Furthermore, building blocks 80 μm in length, are piled over as in a 2-D pyramid by MTBs to demonstrate microassembly with bacteria [22].

Moreover, Uenoyma and Mitada [23] demonstrated that it is possible to neutralize a living natural microswimmer, e.g., M. Mobile, to eliminate toxic side effects, while keeping the...
cell wall and bacterial motor intact. They confirmed that, with a series of chemicals introduced in the environment, the bacterial motor can be reactivated. Experimental studies are reported on triggering and controlling the rotation rate of the flagella by introducing ions and chemicals to directly intervene the operation of the bacterial motor of certain species [24], [25]. An additional reported method of bacterial maneuvering is an application of small electric currents to change the speed and direction of wave propagation [26]. The ability to control the swimming velocity and direction of natural micro/nanoswimmers indicates the need for reliable real-time analytical models.

Comprehensive mathematical models on the propulsion of microorganisms have been around for over 60 years. Hancock [27], using the slender body theory (SBT), formulated the resistive force theory (RFT) for particles undergoing quasi-static rigid-body motions in low Reynolds number viscous flows. In the RFT method, fluid force vector acting on a moving object is linearly proportional to the rigid-body velocity vector relative to the stationary fluid. However, the RFT model leads to omission of body–tail interactions: resistive force coefficients are based on local translations of slender tails [28], [29] and rigid-body motions of isolated bodies with well-known geometries [30], [31].

Keller and Rubinow [32] presented a total six degrees-of-freedom ( dof) analytical model for natural microswimmers and pointed out that the local fluid resistance on a moving and deforming object of arbitrary shape is effected by the entire induced flow field. De la Torre and Bloomfield [33] modeled a representative microswimmer as a series of spherical bodies and studied the local effects of body–tail interactions on the rotating tail by HI tensors. The authors concluded that the local hydrodynamic forces acting on the tail differ dramatically near the joint between body and tail due to the cross interactions. Johnson [34] discussed that the SBT method analysis of helical swimmers presents nonzero lateral forces based on the HIs between swimmer’s body and tail. Watari and Larson [35] discussed that the instantaneous flow field induced around a natural swimmer demonstrates transient behavior and the time average of the flow-field strength is smaller than its instantaneous magnitude. The authors added that the hydrodynamic force on the swimmer’s body is also influenced by induced flow fields. The aforementioned conclusions point out that the stationary fluid assumption is not accurate in the calculation of the drag force on the body.

Phan-Thien et al. [36] used the boundary-element method (BEM) to solve Stokes equation and studied the effects of the geometry of the helical tail and the geometry of a spheroid body on the forward velocity and hydrodynamic efficiency of the microswimmers. The authors discussed that the interaction between the two links decreases forward swimming velocity and the hydrodynamic efficiency of the swimmer. Ramia et al. [37] carried out BEM analysis to obtain the motion of spheres with a single rotating helical tail that is swimming in unbounded and bounded fluids. They studied the effect of HI on the overall propulsive and resistive behavior of the helical tail separately in detail. In both studies, the main focus was on the forces that are acting on the helical tail, swimming velocities, and hydrodynamic efficiency. It was concluded that the overall forward drag resistance of the swimmer increases with HIs.

Hydrodynamic models are of great importance because they are also used in the determination of geometric properties and swimming trajectories for bacteria and spermatozoa species. The RFT approach is employed to determine the high-order plane-wave form and to predict the motion of spermatozoa cells in full motion based on observations [38]. Planar wave actuation is more advantageous to investigate by a high-speed-and-resolution camera since the resultant motion is typically confined to the plane in which wave propagation takes place. However, tracking or observation of a bacterial cell in the third dimension proposes a more challenging task due the dimensions, thus observations on cells presented in the literature are mostly limited to constrained plane motions [39], [40], although there exists recent 3-D-tracking examples for protists [41], [42]. Furthermore, 3-D trajectory construction studies are carried out with solutions of stochastic differential equations based on the observations on 2-D motion [43].

In addition to trajectory construction studies, the RFT is formerly employed in order to predict the propulsive forces generated by a number of artificial helical swimmers in nanometer-, micrometer-, millimeter-, and centimeter-scale subject to various swimming conditions [44]–[49]. In a recent study, Mahoney et al. [47] utilized an RFT-based hydrodynamic model in order to predict necessary hydrodynamic forces in real-time and effectively control the velocity of a magnetically actuated millimeter-length helical swimmer with gravity compensation in an open-loop control scheme.

Furthermore, previous studies confirm that, as long as the inertial forces are significantly dominated by the viscous forces within the fluid, i.e., $Re < 0.1$, the RFT approach is capable of predicting the time-averaged spatial velocities of an untethered swimmer, with an acceptable error, regardless of its actual size [48]–[50]. However, it is verified by Higdon [51] that power consumption of a microswimmer is miscalculated by the RFT method.

B. Main Contributions

Numerical studies conclude that the HI between the body and helical tail is significant; but, a comprehensive analysis to quantify the drag force on the body in the presence of an actuated tail is not presented in the literature to the best of our knowledge. Furthermore, the lateral oscillations of the bacteria are not considered kinematically in analytical models so far. Given the complicated shape of the body–tail assembly and the HIs between them, conventional diagonal resistance matrix approach for isolated axisymmetric rigid particles in viscous flows is insufficient to account for the lateral oscillations of bacteria.

In this study, a computational fluid dynamics (CFD) model, which is validated with vertical in-channel swimming experiments on centimeter-scale bacteria-like robots, is employed to examine the 4-dof motion of a biomimetic swimmer comprised of a rotating rigid helical tail and a spherical body, which are held together with a revolute joint. Experiments are designed
to eliminate all known physical phenomena, e.g., forces such as Brownian noise, which is of importance in nanoscale [12], gravitational pull, and lubricated friction, but far-field HIs that are acting on the wet surfaces.

Initially, using the CFD model, we studied swimming velocities with induced flow fields and obtained the hydrodynamic forces that are acting on the swimmer surface. Subsequently, we employed complex-impedance analysis in the RFT model to introduce HI coefficients, which are embedded in the resistance matrix, to compensate for the flow-field interactions and predict the instantaneous fluid resistance accurately for viscous swimming conditions regardless of the dimensions of bacteria or bacteria-like robots. It is verified that modified resistance matrix predicts time-dependent fluid forces with superior precision. Moreover, the effect of the body and tail geometry is studied concluding that the HI is vastly dominated by the latter determining the swimming trajectory.

II. METHODOLOGY

A. Resistive Force Theory Model

The RFT approach is well documented in [11], [27]–[29], and [32]: in the Reynolds number or creeping flow regime, the fluid resistance $F_r$, i.e., the drag force, which is acting on the moving particle along an arbitrary axis is linearly proportional to the velocity $V_j$ of that particle. This is a valid approach to predicting the drag force per unit length on a deformed slender body submerged in a highly viscous fluid with $Re < 0.1$ [28], [29]. Furthermore, the total fluid drag on a submerged particle freely moving in a viscous flow should add up to zero [52]. Using these two linear relationships, one can write down the equation of motion for a two-link helical swimmer as follows:

$$ F_b + F_t = 0 $$
$$ F_{(b,t)} = -B_{(b,t)}V_{(b,t)} $$

where $B$ denotes the fluid resistance matrix for each link, namely body and tail denoted by the subscripts “$b$” and “$t$”, respectively.

Tail resistance $B_t$ is obtained integrating the local force coefficients, which are projected onto the lab coordinates with the local frame rotations, over the actual chord length $\ell$ in the following fashion:

$$ B_t = \int_\ell \begin{bmatrix} R & R^T & -R & R^T & S & S^T \end{bmatrix} d\ell $$

where $R$ is the rotation matrix between local Frenet–Serret frames and swimmer frame [53] [see Fig. 1(a)], $S$ is the skew-symmetric matrix corresponding to the cross product with the time-dependent position vector $P$, $C$ signifies the local fluid resistance matrix of the tail, and the superscript “$T$” denotes the matrix transpose.

The position vector on a rotating left-handed helical tail with wavelength $\lambda$, angular rotation $\omega$, and local amplitude $B(x)$ for an arbitrary $x$-position can be specified by

$$ P = [x \quad B(x)\cos(\omega t - kx) \quad B(x)\sin(\omega t - kx)]^T $$

The local amplitude is given by $B(x) = B_0 \min(1, \chi/0.1)$, where the position ramp function marks the converging end of the helical tail of length $L$ with $\chi$ denoting the normalized $x$-position along the tail. The maximum possible amplitude is indicated by $B_0$, and $k$ in (4) signifies the wavenumber as $k = 2\pi/\lambda$. Rotational velocity of the tail is given by $\omega = \Omega \times \mathbf{P}$ with the rotation rate of $\Omega = [\omega_x \ 0 \ 0]^T$.

The local fluid resistance on the tail, denoted by $C$ in (3), is a diagonal matrix that consists of the resistance coefficients in the tangent, normal, and binormal directions. The coefficient set preferred in this text is [29]

$$ c_{r} = \frac{2\pi\mu}{\ln(0.18\lambda/\alpha r_1)} $$
$$ c_{(n,b)} = \frac{4\pi\mu}{\ln(0.18\lambda/\alpha r_1) + 0.5} $$

where $\mu$ is the dynamic viscosity, $r_1$ is the tail radius, and $\alpha$ is the ratio of tail length to chord length, i.e., $\alpha = L/\ell$.

The resistance matrix $B_b$ for the rigid body in (2) is

$$ B_b = \begin{bmatrix} D & G \\ G^T & E \end{bmatrix} $$

where $D$ and $E$ are $3 \times 3$ matrices indicating the translational and rotational resistances of the body, respectively. The off-diagonal $G$ matrix in (7) is zero if center of mass of the axisymmetric body lies along the long-axis of the swimmer. In this study, the resistance coefficients presented in [30] are used in analytical calculations. For an axisymmetric body, $D$ and $E$ are conventionally considered diagonal matrices; for a spherical body, the
where $\mathbf{B}_s$ is the effective fluid resistance matrix of the entire swimmer [48], [49]. Furthermore, one may impose “0” on all elements of any row and column in $\mathbf{B}_s$ to eliminate translational or rotational motion along a desired axis.

### B. Computational Fluid Dynamics Model

Fig. 1(b) demonstrates the microswimmer in the time-dependent fluidic domain $\Phi(t)$ bounded by the cylindrical channel. Consider a spherical body with a helical tail. One end of the helical tail is converging to its long axis, where the revolute joint is placed. This geometric design is a valid representation for some bacteria species [50]. The spherical body and a helical tail are apart from each other with the tail radius in order to eliminate discontinuity under angular velocity boundary conditions. It is considered that both body and helical tail are neutrally buoyant with the surrounding medium, which is bounded by a cylindrical channel. The channel diameter is ten times that of the sphere diameter to eliminate the wall effects [54], and the swimmer is placed coaxially, as shown in Fig. 1(b).

Time-dependent incompressible Navier–Stokes equations govern the induced flow field in $\Phi(t)$ and are subject to continuity as follows:

$$
\rho \left( \frac{\partial \mathbf{U}}{\partial t} + (\mathbf{U} - \dot{x}_{\text{mesh}}) \cdot \nabla \mathbf{U} \right) = -\nabla p + \mu \nabla^2 \mathbf{U} \quad (9)
$$

$$
\nabla \cdot \mathbf{U} = 0. \quad (10)
$$

Here, $\mathbf{U}$ and $\dot{x}_{\text{mesh}}$ are respective fluid and mesh velocity vectors computed in $\Phi(t)$, $\rho$ is the fluid density, and $p$ denotes the hydrostatic pressure. Mesh of the swimmer is handled with arbitrary-Lagrangian-Eulerian (ALE) deformation in order to incorporate motion of swimmer boundaries with respect to stationary channel walls [55].

Zero-velocity and zero-pressure initial conditions are set for (9) and (10) initially, whereas no-slip boundary condition is imposed on stationary channel walls at all times. Normal stress vectors are set to zero at channel’s inlet and outlet to achieve open-flow boundary condition [56].

Position vector on the rotating left-handed helical tail is signified with a modified local amplitude function as $\mathbf{B}(x) = \mathbf{B}_h \min(1, \chi/0.1 \min(1, f/4t))$, where $f$ denotes the actuation frequency of the tail. The local amplitude increases with a time ramp to ensure smooth transition of the fully developed rotating helical profile for the surrounding fluid.

Resultant body rotation rate vector, due to conservation of angular momentum, is given as $\Omega_b = [\Omega_x, 0, 0]^T$, and the corresponding fluid and mesh velocity boundary conditions on the surfaces of body, i.e., $\Psi_b$, and on the surfaces of tail, i.e., $\Psi_t$, are given respectively by

$$
\mathbf{U} = \mathbf{V} + \Omega_b \times \mathbf{x}_s \quad \iff \mathbf{x}_s \in \Psi_b \quad (11)
$$

$$
\mathbf{U} = \mathbf{u} = \frac{d\mathbf{P}}{dt} + \mathbf{V} \quad \iff \mathbf{x}_s \in \Psi_t \quad (12)
$$

where $\mathbf{x}_s$ signifies the position vector of an arbitrary point on the surface of the swimmer with respect to its center of mass.

Resultant swimming velocity vectors are computed with force-free-swimming constraints: in creeping flows, the fluid resistance on the entire surface of a self-propelling swimmer adds up to zero [52]. Thus, the total instantaneous fluid force is set to zero in order to obtain rigid-body velocities satisfying zero-net-force and zero-net-torque constraints. The respective constraint equations for the hydrodynamic force and hydrodynamic torque that are on the entire surface of the swimmer are specified as follows:

$$
\int_{\Psi_b + \Psi_t} \left[ -p\mathbf{I} + \tau \right] \mathbf{n} \, dA = 0 \quad (13)
$$

$$
\int_{\Psi_b + \Psi_t} \mathbf{x}_s \times \left[ -p\mathbf{I} + \tau \right] \mathbf{n} \, dA = 0. \quad (14)
$$

Here, $A$ denotes the surface area in contact with the viscous fluid, local surface normal vector is signified by $\mathbf{n}$, and $\tau$ stands for the viscous stress tensor. Initial conditions are $\mathbf{V} = 0$ and $\Omega_b = 0$; the constraint equations are solved at each time increment based on the fluid resistance corresponding to the resultant rigid-body velocities of the preceding time-step combined with the tail rotation already in progress.

The last two rows of the constraints (13) and (14) are excluded in the CFD model and the lateral rigid-body rotations, i.e., yaw and pitch, are eliminated. Omission of lateral rotations of the swimmer frame in the channel frame greatly simplifies the mesh deformation in $\Phi(t)$ eliminating numerical convergence issues and rotation matrix calculations between the two frames. Furthermore, Hyon et al. [57] studied wiggling trajectories of bacteria and concluded that lateral rotations of the swimmer are observed clearly when the tail is not collinear with the symmetry axis. Otherwise, relatively straight trajectories are observed owing to much faster rate of rotation of the tail compared with the body [57].

### C. Experiments

In this study, a set of in-channel experiments, which are reported in detail elsewhere [49], are used to validate the CFD model. A centimeter-scale biomimetic robot comprising of a cylindrical body and a rigid helical tail, which is actuated by a dedicated dc-motor, is used in experiments [see Fig. 2(a)]. One end of the rigid tail is deformed with a hyperbolic-tangent profile and attached to the rotor of the dc motor, which constitutes the revolute joint allowing body and tail to rotate in opposite directions in order to mimic swimming of a bacterium with a single helical tail [50].
Fig. 2. Experimental setup. (a) Bioinspired robot consisting of a cylindrical body and helical tail. (b) Robot inside a filled glass channel (no cork). (c) Robot, with a cylindrical cork glued on the tip, swimming vertically.

<table>
<thead>
<tr>
<th>Dimensions</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Channel Diameter, $2R_b$</td>
<td>35 mm</td>
</tr>
<tr>
<td>Channel Length, $L_b$</td>
<td>350 mm</td>
</tr>
<tr>
<td>Glass Body Diameter, $D_{cc}$</td>
<td>18 mm</td>
</tr>
<tr>
<td>Copper Wire Diameter, $2r_t$</td>
<td>1 mm</td>
</tr>
<tr>
<td>Total Body Mass</td>
<td>11 g</td>
</tr>
<tr>
<td>Li-Po Pack Rating</td>
<td>70 mAh with 3.7 V</td>
</tr>
<tr>
<td>Si-Oil Density</td>
<td>985 kg/m³</td>
</tr>
<tr>
<td>Si-Oil Viscosity</td>
<td>3.5 Pa·s</td>
</tr>
<tr>
<td>CCD-Camera Specs</td>
<td>640-by-480 Pixels @ 30-fps</td>
</tr>
</tbody>
</table>

The body of the biomimetic robot, which is a glass tube 18 mm in diameter [see Fig. 2(b)], houses a dc motor, a Li-Po battery pack, and a driver circuitry with IR receiver to achieve remote control of motor actuation. A cylindrical cork is glued at the tip of the body to obtain neutral buoyancy and ensure stable swimming in the opposite direction to the gravitational pull without surface contact, and to restrict rigid-body rotations along the lateral directions by applying a restoring torque [see Fig. 2(c)]. Properties of the biomimetic robot are listed in Table I.

![Diagram](image)

### III. RESULTS

#### A. Resistive Force Theory Model Versus Observations

The RFT model is validated with the forward velocity and body rotation rate reported for certain bacteria species by Chattopadhyay and Wu [50]. The authors compared the effectiveness of SBT and RFT methods against the time-averaged forward velocities and body rotation rates observed in their own experiments with *V. Alginolyticus*, *C. Crescentus*, and *E. Coli* minicell concluding that the former is more accurate in all cases [50]. It is noted that although some of the cell dimensions are close to or smaller than 1 μm, analytical approximation methods, which only incorporate local flow fields or local resistance coefficients, are still reliable.

Here, the RFT method is employed to ascertain the necessary corrections on the resistance coefficients of the axisymmetric bodies of the species, whose dimensions and wave properties are presented in Table II. Solutions are carried out by the Adams–Bashforth–Moulton PECE solver [58] and average velocities are obtained over one complete period. The reported [50] and calculated velocity values and the determined correction factors to assure less than 0.1% error for RFT-model predictions are presented in Table III.

![Diagram](image)

### Table II

<table>
<thead>
<tr>
<th>Species</th>
<th>$f$ (Hz)</th>
<th>$B_v$ (nm)</th>
<th>$\lambda$ (μm)</th>
<th>$L$ (μm)</th>
<th>$r_i$ (nm)</th>
<th>$D_b$ (μm)</th>
<th>$D_{b,cl}$ (μm)</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>V. Alginolyticus</em></td>
<td>571</td>
<td>140</td>
<td>1.2</td>
<td>3.7</td>
<td>16</td>
<td>4.6</td>
<td>0.7</td>
</tr>
<tr>
<td><em>C. Crescentus</em></td>
<td>311</td>
<td>140</td>
<td>0.96</td>
<td>4.5</td>
<td>7</td>
<td>1.92</td>
<td>0.84</td>
</tr>
<tr>
<td><em>E. Coli</em> minicell</td>
<td>78</td>
<td>190</td>
<td>2.3</td>
<td>6.2</td>
<td>12</td>
<td>0.82</td>
<td>0.82</td>
</tr>
</tbody>
</table>

### Table III

<table>
<thead>
<tr>
<th>Observation</th>
<th>RFT Calculation</th>
<th>Corrections</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U_f$ (μm/s)</td>
<td>$\Omega_f/2\pi$ (Hz)</td>
<td>$\tau_{r,T}$ (μs)</td>
</tr>
<tr>
<td><em>V. Alginolyticus</em></td>
<td>34</td>
<td>26</td>
</tr>
<tr>
<td><em>C. Crescentus</em></td>
<td>30</td>
<td>31</td>
</tr>
<tr>
<td><em>E. Coli</em> minicell</td>
<td>14</td>
<td>31</td>
</tr>
</tbody>
</table>

Results point out that the resistance coefficients provided for an isolated axisymmetric blunt object are inadequate to predict the hydrodynamic forces and torques that are acting on its surface. The need for further study on the induced flow fields around helical micro/nanoswimmers in order to ascertain the cause of this discrepancy is clearly indicated.

### B. Validation of Computational Fluid Dynamics Model With Experiments (Using Actual Dimensions)

Experimental studies are carried out on four different tails with different amplitude and wavelength values. Each experiment is repeated a total of five times and forward velocity values are obtained from captured images. Error bars illustrated...
in Fig. 3 are obtained with 95% confidence interval. The CFD simulations are carried out with actual dimensions and physical properties with \( \Phi(t) \) being discretized with second-order Lagrangian tetrahedral elements. Governing equations and force-free-swimming constraints are handled with PARDISO linear solver [59].

Fig. 3 demonstrates that the CFD model predicts the effect of varying wave geometry on the forward swimming velocities reasonably well. Wave amplitude attains two distinct values, i.e., \( B_0 = \{ 4.5, 4.5, 7.5, 7.5 \} \) mm, whereas each helical tail has a different wavelength, i.e., \( \lambda = \{ 12, 16, 11, 15 \} \) mm with different apparent lengths \( L = \{ 60, 93, 42, 56 \} \) mm, respectively. Observed respective actuation frequencies for specified wave and tail geometries are \( f = \{ 0.909, 0.937, 0.569, 0.569 \} \) Hz, with an error interval of \( \pm 0.01 \) Hz. The respective maximum and minimum errors are, respectively, 13.6% and 8.8% in the forward velocity predictions, whereas 12.5% and 25% in body rotation rates. Forward swimming [see Fig. 3(a)] and body rotation rate [see Fig. 3(b)] results are presented in translational velocity ratio, i.e., \( V_x/\dot{x} \), and in rotational velocity ratio, i.e., \( \Omega_z/\omega \), with respect to different wavenumbers.

C. Validation of Computational Fluid Dynamics Model With Observations on the E. Coli Minicell (Using Dimensionless Analysis)

Dimensionless analysis, which is summoned in the following sections extensively, is a common practice in numerical investigations on micro/nanoswimmers [36], [37], [60], [61]. Furthermore, CFD models benefit dimensionless-study approach with viscous flow regimes provided that suitable characteristic length- and time scales are used [62].

Employing the computational model presented here, but with a channel diameter ten times that of the spherical body, we simulated nanoscale species \( E. \) Coli minicell [50] that is swimming fully submerged in a large aquatic medium at room temperature in order to demonstrate that the accuracy does not deteriorate with the dimensionless analysis.

The CFD model is validated by means of observed geometric properties and calculated scaling constants [see Table IV]: spherical body diameter is the length scale, \( f \) is the time scale, and Reynolds number is \( Re = \rho D_b^2 f / \mu \); therefore, dimensionless values used in the CFD model are \( D_x = 1, L = 7.56, r_t = 0.0146, B_0 = 0.231, \lambda = 2.804, \rho = 1, f = 1, \) and \( \mu = 21376 \), with velocity scaling factors \( V_{scale} = 63.96 \mu m/s \) and \( \Omega_{scale} = 78 \) Hz. The CFD model predicts \( V_x = 0.194 \) and \( \Omega_z/2\pi = 0.3647 \). Thus, the equivalent dimensional velocities are \( V_x = 12.408 \mu m/s \) and \( \Omega_z/2\pi = 28.453 \) Hz.

Respective errors in the CFD model prediction are 11.37% and 8.21% for forward velocity and body rotation rate compared with the observations [50]. Low error values with a nanoscale body and tail radii, thus with the likely presence of considerable Brownian noise [12], suggest that the model is sound. However, the CFD model is primarily validated with the results of the centimeter-scale experiments because achieving individual control on the tail and wave parameters in nanoscale while keeping the body geometry fixed is unfeasible.

D. Swimmer Trajectory and Flow Fields Induced by the Tail Rotation

The governing equations (9) and (10) are cast in nondimensional form in the following flow-field study; with the diameter of the body, \( D_b \) as the length scale and \( 2\pi/\omega \) as the time scale, and hence, \( D_b \omega/2\pi \) as the velocity scale. Therefore, the scaling Reynolds number is \( Re = \rho D_b^2 \omega/2\pi \). The Scaling Reynolds number used in the CFD model is set to \( 10^{-2} \) to ensure creeping flow conditions. A complete list of variables used in the dimensionless base-case CFD simulation is presented in Table V.

Second-order Lagrangian tetrahedral elements are used in CFD studies and the helical tail of the swimmer is discretized homogeneously resulting in 300,000 dof. The linear system of equations is solved with the PARDISO linear solver [59] and a second-order backward difference formula with variable time stepping for numerical integration with the maximum

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Dimensional Value [50]</th>
<th>Dimensionless Value (CFD)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_x )</td>
<td>820 nm</td>
<td>1</td>
</tr>
<tr>
<td>( r_t )</td>
<td>12 nm</td>
<td>0.0146</td>
</tr>
<tr>
<td>( L )</td>
<td>6.2 ( \mu m )</td>
<td>7.56</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>2.3 ( \mu m )</td>
<td>2.804</td>
</tr>
<tr>
<td>( B_0 )</td>
<td>190 nm</td>
<td>0.231</td>
</tr>
<tr>
<td>( f )</td>
<td>78 Hz</td>
<td>1</td>
</tr>
<tr>
<td>( \rho )</td>
<td>1000 kg/m(^3)</td>
<td>1</td>
</tr>
<tr>
<td>( Re )</td>
<td>4.678\times10^{-5}</td>
<td>4.678\times10^{-4}</td>
</tr>
<tr>
<td>( \mu )</td>
<td>10( ^{-2} ) Pa.s</td>
<td>21376</td>
</tr>
<tr>
<td>( V_{scale} )</td>
<td>63.96 ( \mu m/s )</td>
<td>1</td>
</tr>
<tr>
<td>( \Omega_{scale} )</td>
<td>78 Hz</td>
<td>1</td>
</tr>
<tr>
<td>( V_x )</td>
<td>14 ( \mu m/s )</td>
<td>0.194</td>
</tr>
<tr>
<td>( \Omega_z/2\pi )</td>
<td>31 Hz</td>
<td>0.3647</td>
</tr>
</tbody>
</table>
TABLE V
PARAMETERS FOR THE BASE-CASE CFD SIMULATION

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter Name</th>
<th>Dimensionless Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_b$</td>
<td>Spherical Body Diameter</td>
<td>1</td>
</tr>
<tr>
<td>$r_t$</td>
<td>Cylindrical Tail Radius</td>
<td>0.05</td>
</tr>
<tr>
<td>$L_t$</td>
<td>Cylindrical Tail Length</td>
<td>2</td>
</tr>
<tr>
<td>$\lambda_t$</td>
<td>Wave Length</td>
<td>2/3</td>
</tr>
<tr>
<td>$B_a$</td>
<td>Wave Amplitude</td>
<td>0.1</td>
</tr>
<tr>
<td>$f$</td>
<td>Propagation Frequency</td>
<td>1</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Fluid Density</td>
<td>1</td>
</tr>
<tr>
<td>$Re$</td>
<td>Scaling Reynolds Number</td>
<td>$10^7$</td>
</tr>
<tr>
<td>$\mu/1/Re$</td>
<td>Fluid Viscosity</td>
<td>100</td>
</tr>
<tr>
<td>$L_{ch}$</td>
<td>Cylindrical Channel Length</td>
<td>10</td>
</tr>
<tr>
<td>$2R_{ch}$</td>
<td>Cylindrical Channel Diameter</td>
<td>10</td>
</tr>
</tbody>
</table>

The rigid-body velocity of the microswimmer in $xyz$-frame is illustrated in Fig. 4. Forward velocity $V_x$ [see Fig. 4(a)] and body rotation rate $\Omega_x$ [see Fig. 4(c)] reach to a steady value as the initial ramp is completed while the mesh is deformed to the extend where the local amplitude attains its maximum throughout the tail. Lateral velocities have out-of-phase sinusoidal behavior with zero time average. The instantaneous lateral velocity is always comparable with the forward velocity, and the $\pi/2$ phase between $V_y$ and $V_z$ [see Fig. 4(b)] indicates helical trajectory in $\Phi(t)$.

Fig. 4. Time-dependent velocity vector of the center of mass. (a) Forward velocity, i.e., along $x$-axis. (b) Lateral velocities. (c) Body rotation rate, i.e., along $x$-axis.

dimensionless time step set to 0.025. Computations require approximately 20 h on a high-end workstation to complete three full-periods of the tail rotation.

The rigid-body velocity of the microswimmer in $xyz$-frame is illustrated in Fig. 4. Forward velocity $V_x$ [see Fig. 4(a)] and body rotation rate $\Omega_x$ [see Fig. 4(c)] reach to a steady value as the initial ramp is completed while the mesh is deformed to the extend where the local amplitude attains its maximum throughout the tail. Lateral velocities have out-of-phase sinusoidal behavior with zero time average. The instantaneous lateral velocity is always comparable with the forward velocity, and the $\pi/2$ phase between $V_y$ and $V_z$ [see Fig. 4(b)] indicates helical trajectory in $\Phi(t)$.

Studies on the induced flow field reveal that body and tail experience a mutual HI. A rotating but otherwise anchored helical tail that is submerged in viscous fluids would act as a pump [63]; but, if the anchoring force is released, the momentum exerted on the surrounding viscous domain is transformed into thrust partially. Given the fact that the wave propagation velocity is bigger than the propulsion velocity, the rotating tail would propel itself while pushing the flow on the opposite direction. Thus, the mechanical energy transferred into the surrounding fluid is dissipated simultaneously by the hydrodynamic drag due to resultant swimming action and by the forced flow in the direction of wave propagation due to the pump effect.

In order to single out the influence of tail rotation, translating and rotating bodies with nonrotating and rotating tails are studied, separately. First, a time-dependent velocity vector, which is identical to that obtained from the base-case CFD model [see Fig. 4], is imposed on the surface of a spherical body with a nonrotating helical tail that is attached on the right-hand side, as presented in Fig. 5(a). Boundary conditions on the nonrotating helical tail are set identically to that of the spherical body except for the rigid body rotation, thus the entire swimmer is being dragged through the unbounded viscous fluid. The streamlines that depict the flow field around the sphere become sparser signifying a decrease in viscous stresses especially at the back of the spherical body.

However, when the helical tail is allowed to rotate with an angular velocity of $\omega$ on its long axis, the streamline density behind the body increases considerably [see Fig. 5(b)]. This phenomenon is, in effect, a substantial increase in the velocity gradient due to normal stress build up at the back of the spherical body. The streamlines that depict the flow field around the sphere become sparser especially at the back of the spherical body.

In order to single out the influence of tail rotation, translating and rotating bodies with nonrotating and rotating tails are studied, separately. First, a time-dependent velocity vector, which is identical to that obtained from the base-case CFD model [see Fig. 4], is imposed on the surface of a spherical body with a nonrotating helical tail that is attached on the right-hand side, as presented in Fig. 5(a). Boundary conditions on the nonrotating helical tail are set identically to that of the spherical body except for the rigid body rotation, thus the entire swimmer is being dragged through the unbounded viscous fluid. The streamlines that depict the flow field around the sphere become sparser signifying a decrease in viscous stresses especially at the back of the spherical body.
Based on the HI mediated by the induced flow field, it is concluded that the hydrodynamics of a swimmer’s body is influenced by the rotation of its tail. In the next section, it is observed that the fluid resistance on the body greatly depends on the wave geometry. Additionally, the reader may find a detailed study on the effect of body shape in [65] where the authors investigated the case of bacteria moving next to plane boundaries using BEM analysis, which is beyond the scope of this study, and concluded that the body shape is of importance for stable swimming trajectories.

E. Time-Dependent Hydrodynamic Forces on Body, and the Hydrodynamic-Interaction Coefficients

In this section, we incorporated cross interactions due to the induced flow fields by respective correction coefficients in the fluid resistance matrix $\mathbf{D}$ modified by casting the complex-impedance analysis in the form of amplitude correction and phase-angle correction.

Necessary amplitude corrections for the HI, i.e., $\Upsilon_T$ for rigid-body translation and $\Upsilon_R$ for rigid-body rotation, are calculated based on the ratio of hydrodynamic force obtained by the CFD model to the viscous sphere drag formulae presented in the literature as follows for translation and rotation, respectively

$$
\Upsilon_{T,j} = \begin{cases} 
F_{j,\text{avg}} / D_{T,j} V_{j,\text{avg}} & \text{if } j = x \\
F_{j,\text{max}} / D_{T,j} V_{j,\text{max}} & \text{if } j = \{y, z\}
\end{cases}
$$

$$
\Upsilon_{R,j} = T_{j,\text{avg}} / D_{R,j} \Omega_{j,\text{avg}} \quad \text{if } j = x.
$$

Here, $F_{j,\text{avg, max}}$ denotes the time averaged and maximum normal force acting along an arbitrary axis, which is obtained by integrating total hydrodynamic stresses over the surface of the body in that direction. Similarly, $T_{j,\text{avg}}$ denotes the time-averaged viscous torque exerted on the surface of the swimmer’s body along an arbitrary axis.

Time-dependent hydrodynamic force plots [see Fig. 7] illustrate that a simple correction based on the force to velocity ratio given by (15) and (16) is inadequate to predict the instantaneous lateral hydrodynamic resistances acting on the body. Fig. 7 demonstrates that there exists a constant phase shift between analytical lateral drag forces and the ones obtained by the CFD model: the phase shift, in effect, is between swimming velocities and the hydrodynamic drag, in lateral directions.

The conventional diagonal drag-force coefficient matrix signifies a one-to-one relationship between elements of the velocity vector and respective fluid resistances for an isolated particle undergoing rigid-body translations without any cross interactions. However, to account for the apparent phase shift [see Fig. 7], one may model the instantaneous lateral velocity and instantaneous lateral force vectors in complex planes, with respective amplitudes of $V$ and $F$, as follows:

$$
\begin{bmatrix}
F_y \\
F_z
\end{bmatrix} = \begin{bmatrix}
F \exp(i\omega t) \exp(i\phi) \\
F \exp(i\omega t) \exp(i\phi) \exp(i\pi/2)
\end{bmatrix}
$$

$$
V_y + V_z = V \exp(i\omega t).
$$

Thus, the elements of the conventional drag-force coefficient matrix in the RFT model are modified in order to compensate...
for the HI effects in the time domain, and nonzero off-diagonal terms are introduced to account for the cross interactions, which lead to an unsymmetrical and orthogonal matrix, as follows:

\[
F_0(\phi) = \begin{bmatrix}
D_{T,x} T_{T,x} & 0 & 0 \\
0 & D_{T,y} T_{T,y} \cos(\phi) & D_{T,y} T_{T,y} \sin(\phi) \\
0 & -D_{T,z} T_{T,z} \sin(\phi) & D_{T,z} T_{T,z} \cos(\phi)
\end{bmatrix} V,
\]

where the phase-angle \( \phi \), for the spherical body, is obtained from Fig. 7 by solving the inverse problem for the phase shift.

The forward rigid-body translation in (19) does not require phase-angle correction because the normal-force build up at the back of the body is a steady effect due to continuous rotation of the helical tail. Similarly, the hydrodynamic \( x \)-torque that is acting on the body in (7) is also constant in time. The predicted HI coefficients, amplitude correction, and the phase-angle, for the base-case CFD model, are presented in Table VI.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter Name</th>
<th>Predicted Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Upsilon_{T,x} )</td>
<td>HI-coefficient for ( x )-force</td>
<td>2.24</td>
</tr>
<tr>
<td>( \Upsilon_{T,(y,z)} )</td>
<td>HI-coefficient for lateral force</td>
<td>0.51</td>
</tr>
<tr>
<td>( \Upsilon_{T,z} )</td>
<td>HI-coefficient for ( x )-torque</td>
<td>1.09</td>
</tr>
<tr>
<td>( \phi )</td>
<td>Phase-angle</td>
<td>1.17( \pi )</td>
</tr>
</tbody>
</table>

TABLE VI
PREDICTED HI COEFFICIENTS AND PHASE-ANGLE FOR THE BASE-CASE CFD MODEL

The main reason for this change in behavior is incomplete waves: with full waves, the \( V_{y,z} \) components of the swimming velocity are small, thus the body does interact with the induced flow field minimally. On the other hand, incomplete waves induce lateral thrust and swimmer body moves sideways that lead to further interaction with the surrounding flow field. A similar local minima and maxima relation is observed between \( \Upsilon_{R,x} \) and \( N_3 \): the variations are negligible and the overall relation can be practically deemed as linear; however, inversely proportional to varying \( N_3 \) as presented in Fig. 8(c).

The relationship between \( \Upsilon_{T,z} \) and wave amplitude is linear: the normal stress that is acting on the hemispherical surface on the right-hand side of the body increases with increasing \( B_z \), akin to increasing \( N_3 \) [see Fig. 9(a)]. The amplitude correction of lateral HI coefficient in lateral directions \( \Upsilon_{T,(y,z)} \), also varies linearly with wave amplitude; however, the amplification effect is significantly low [see Fig. 9(b)]. Finally, \( \Upsilon_{R,x} \) is inversely proportional to the wave amplitude, and varies slightly converging to 1 as \( B_z \) increases [see Fig. 9(c)]. Hence, the body is less affected by the tangential component of the flow field induced by the counter rotation of the tail.

The base-case CFD simulation computes a 1.17\( \pi \) phase-angle for the helical tail with \( N_3 = 3 \) and \( B_z = 0.1 \) as given in Table VI. Phase-angle dips to local minima for wavelengths shorter than half-wave on the tail, i.e., including quarter of a wavelength such as \( N_3 = \{0.25, 1.25, 2.25, 3.25, \ldots\} \) to be exact [see Fig. 10(a)]. Local minima of phase-angle coincide with the local maxima of amplitude correction in lateral directions, as depicted by Figs. 8(b) and 10(a). Moreover, the phase-angle reaches to local maxima with the presence of half waves, i.e., \( N_3 = \{0.5, 1.5, 2.5, 3.5, \ldots\} \).
Fig. 9. Relation between the amplitude correction of HI coefficients and the helical wave geometry with respect to $B_o$: (a) on the linear translation in $x$-direction with respect to $B_o$; (b) on the linear translation in lateral directions with respect to $B_o$; (c) on the $x$-rotation of the body with respect to $B_o$.

Fig. 10. Effect of wave geometry on phase-angle correction of HI coefficients: (a) with respect to total number of waves on the helical tail $N_\lambda$ and (b) with respect to wave amplitude $B_o$.

Additionally, the phase-angle varies linearly with the wave amplitude $B_o$ as presented in Fig. 10(b). The sensitivity of the phase-angle to the helical wave amplitude is evidently minute.

IV. DISCUSSION

One can make use of an intensive molecular dynamics model to calculate hydrodynamic effects and deduce other forces in micro- and nanoscale experiments. Forces such as Brownian noise and other nanoscale interactions are also important, and must be studied by controlled experiments in micro- and nanoscales: once the HI effects are known, it will be easier to single out other physical phenomena shaping the swimming trajectory of a bacterium.

For instance, it is reported that, the Brownian effect results in change of the swimming direction of E. Coli cells in the long run [12]: the main trajectory is due to the hydrodynamic forces invoked by the wave propagation carried out on the tail; however, Brownian noise happens to introduce a stochastic course alteration approximately every 10 s [12].

We conducted experiments with a centimeter-scale untethered biomimetic robot. Experiments are free of gravitational pull and contact forces. Furthermore, stochastic molecular interactions and electrostatic surface forces completely dilute due to the size of the robotic prototype. Thus, the hydrodynamic effects, which play a major role in the propulsion of micro/nanoswimmers as observed in nature and demonstrated by artificial mechanisms, are effectively isolated. Consequently, the viscous swimming experiments in this study are suitable as to be governed with a simple combination of rigid-body kinematics subject to force-free-swimming constraints and Navier–Stokes equations subject to continuity. Moreover, replicating the experiment in smaller scales is unfeasible due to the impracticality of controlling the tail and wave parameters in micro- and nanoscales.

Without proper HI corrections, body resistance is modeled with a diagonal matrix that calculates the time-averaged velocity vector computed by the CFD model but erroneously: predicted forces and actual forces are out of phase in time domain, thus constructed trajectory and predicted power consumption are incorrect. CFD simulations provide precious information on HIs otherwise could not be easily singled out with mere experiments. The HI phenomenon is explained with the flow-field interactions between the body and the tail, which are modeled with a complex-impedance analogy leading to HI coefficients: with respective amplitude and phase-angle corrections, time-dependent force and velocity vectors are predicted with improved accuracy.

Experimental studies on observation and control of bacterial species will benefit from the improved resistance matrix approach: a biomimetic or cybernetic micro/nanorobot, which is carrying out a predefined task, can be maneuvered successfully in real-time with construction of more accurate 3-D trajectories for control purposes during therapeutic operations, such as targeting cancerous tissue as recently discussed by Felfoul and Martel [18], or some properties of bacteria species that are hard to resolve by mere observation can be determined by the improved kinematic model with the help of time-dependent velocity information, as already demonstrated in the literature via observations on certain spermatozoa species [38].

For instance, the procedure to determine the HI corrections from a conducted controlled experiment with MTBs, provided that all geometric properties are successfully observed, should be in this order. First, one should search for the amplitude-correction factors satisfying the time-averaged forward velocities and the amplitude of lateral velocities. Then, one may find the phase-angle correction via solving the inverse problem for the phase shift between observed and RFT-predicted lateral velocities. Moreover, HI corrections will be useful even with relatively small wave amplitudes with respect to a large body or a bulky cargo being towed given that the $B_o/D_b$ ratio in this
study varies between 0.01 and 0.15. It is also noted that, for two-link helical swimmers, phase-angle and amplitude corrections are not a function of one another.

V. CONCLUSION

Biomimetic micro/nanorobots and single-celled organisms are of great importance for future in vivo and in vitro applications in biomechanics such as minimal invasive surgery. Hence, improved hydrodynamic models based on well-known resistance coefficients will be extremely useful for accurate trajectory generation and control of natural micro/nanoswimmers. Hence, we focused on improving an otherwise well-known deterministic tool.

We conducted dimensionless time-dependent CFD simulations in order to study the flow fields induced by a helical swimmer in viscous domains. We qualitatively studied the effect of the body geometry on the induced flow field: tail rotation amplifies the hydrodynamic stress increasing the spatial streamline density at the back of the spherical body. After examining the flow fields and swimmer trajectory in detail, we quantified the HI between the swimmer’s body and a rotating helical tail by introducing two HI coefficients, i.e., amplitude and phase-angle corrections, based on complex-impedance analysis carried out on the time-dependent hydrodynamic force vector. The modified resistance matrix and the improved RFT model are demonstrated to be indispensable in micro/nanorobotic applications with the ability to predict time dependent force vectors accurately.

Furthermore, we quantitatively studied the relationship between HI coefficients, and the wave geometry. It is demonstrated that the phase-angle of the lateral HI has a nonlinear relationship with total number of waves and mildly sensitive to the wave amplitude: the nonlinear sensitivity to wavenumber indicates the need for further study within a wider design space with higher resolution.

REFERENCES


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