Bistability in the synchronization of actuated microfilaments

Hanliang Guo¹, Lisa Fauci², Michael Shelley³,⁴, and Eva Kanso¹,³,⁴*

1. Aerospace and Mechanical Engineering, University of Southern California, Los Angeles, California, USA
2. Department of Mathematics, Tulane University, New Orleans, Louisiana 70118, USA
3. Center for Computational Biology, Flatiron Institute, Simons Foundation, New York 10010, USA
4. Courant Institute of Mathematical Sciences, New York University, New York, New York 10012, USA

* kanso@usc.edu

ABSTRACT

Cilia and flagella are essential building blocks for biological fluid transport and locomotion at the micron scale. They often beat in synchrony and may transition between different synchronization modes in the same cell type. Here, we investigate the behavior of elastic microfilaments, protruding from a surface and driven at their base by a configuration-dependent torque. We consider full hydrodynamic interactions among and within filaments and no slip at the surface. Isolated filaments exhibit periodic deformations, with increasing waviness and frequency as the magnitude of the driving torque increases. Two nearby but independently-driven filaments synchronize their beating in-phase or anti-phase. This synchrony arises autonomously via the interplay between hydrodynamic coupling and filament elasticity. Importantly, in-phase and anti-phase synchronization modes are bistable and co-exist for a range of driving torques and separation distances. These findings are consistent with experimental observations of in-phase and anti-phase synchronization in the biflagellate Chlamydomonas reinhardtii and could have important implications on understanding the biophysical mechanisms underlying transitions between multiple synchronization modes.
I. INTRODUCTION

Cilia and flagella exhibit synchronous motion. The biflagella of the alga *Chlamydomonas* often beat symmetrically at the same frequency but opposite phase\(^{15,16,36–38}\). Sperm cells tend to synchronize their tail beating in-phase when they are in close proximity\(^{18,46}\). Motile cilia in aquatic organisms and in mammalian tissues coordinate their collective beating in a wavelike pattern\(^{3,4,13}\).

Theoretical models suggest that these modes of synchronization can arise from hydrodynamic coupling between flagella\(^{17,20,30,32,42,43}\), assisted by flagellar elasticity\(^{10,14}\). Existing models are based either on low-order representations of flagella and cilia in the form of ‘bead-spring’ oscillators\(^{6,17,24}\) or on more realistic models of hydrodynamically-coupled elastic filaments\(^{14,23,35}\). These models primarily reproduce one mode of synchrony: anti-phase, in-phase, or metachronal coordination. Flagellar synchrony is more complex: flagella and cilia can exhibit multiple synchronization modes even within a single cell type or organism. For example, the flagella of a *Chlamydomonas* stochastically switch between anti-phase and in-phase synchrony\(^{27,44}\). Cilia in mammalian brain ventricles periodically change their collective beat orientation, providing a cilia-based switch for redirecting the transport of cerebrospinal fluid at regular intervals of time\(^{12}\). The origins of these transitions, whether abrupt and stochastic (*Chlamydomonas* biflagellates) or gradual and periodic (ependymal cilia), are currently unknown.

In models that represent flagella as coupled oscillators driven by a configuration-dependent force, the functional dependence of this force on configuration needs to be altered in order for the system to exhibit a different mode of synchrony (see\(^5\) for review). The need to modify the functional form of the drive, and consequently the landscape of the associated potential field, makes implicit assumptions on the mechanisms responsible for different modes of synchrony. It assumes that these mechanisms induce a fundamental change in the internal machinery that drives the flagellum or cilium beyond what can be captured by rescaling the intensity of the drive. In this study, we present a theoretical model of flow-coupled elastic filaments that exhibits bistable in-phase and anti-phase synchronization at the same drive level, suggesting that the aforementioned assumption is not required to achieve multiple synchronization modes.

The synchronization of filaments in viscous fluid has been studied since the seminal
FIG. 1. (a) Elastic filament actuated by a motor at its base with configuration-dependent bending moment $M_b$. The moment switches direction when the tangent to the base reaches pre-defined target angles $\pm \Theta$. (b) Discretization of the elastic filament into $N + 1$ spheres of diameter $a$. (c) Low-order model of a shape dependent oscillator driven by an applied force $F$ that switches directions once the oscillator reaches a predefined oscillation amplitude $|x| = X_S$.

work of$^{40}$, where he showed that traveling waves in two parallel infinite sheets have the least viscous dissipation when synchronized in-phase. These results were later extended to include waveform compliance$^{10}$ and three-dimensional (3D) beating$^{30,33}$ considered elastic sheets and filaments of finite length and computationally showed that neighboring sheets and filaments with symmetric beating patterns always synchronize in-phase. In-phase synchrony was also predicted by$^{14}$. A model of cilia that tracked the action of a discrete set of molecular motors between two semi-flexible microtubule fibers also demonstrated that neighboring cilia, coupled only through hydrodynamics, quickly synchronize their beat$^{48}$.

$^{24}$ and$^6$ proposed optically-driven colloidal oscillators as a model system for studying synchronization between cilia and flagella. In these systems, the colloidal particle is constrained to move on a linear trajectory under the influence of a driving force that switches direction once the particle approaches pre-defined target positions, hence the name “geometric switch.” Here, we extend the geometric switch model to finite microfilaments submerged in viscous fluid and driven at their base by an active bending moment that switches direction at pre-defined orientations of the tangent at the filament’s base. Our model, although conceived independently, is reminiscent to the model used in$^{23}$ for studying metachronal wave coordination. We find that single filaments exhibit time-periodic deformations that seem to be insensitive to the initial configuration of the filament, and we quantify the consequent frequency of these deformations. We then show that two hydrodynamically-coupled filaments can achieve in-phase and anti-phase synchronizations that are bistable for a range of parameter values. To highlight the main physical mechanisms responsible for these synchronization modes, we introduce a low-order particle model that accounts for elasticity and
shape changes. The simpler model indicates that bistable synchronizations emerge as a result of hydrodynamic-coupling, shape changes and an internal restoring moment due to filament elasticity. We conclude by commenting on the relevance of these results to understanding the biophysical mechanisms underlying transitions between multiple synchronization modes in flagella and cilia.

II. CONTINUUM MODEL

Consider an inextensible elastic filament of length $\ell$ and diameter $a$ rooted at the origin $O$ of a Cartesian coordinate system $(x, y, z)$. Let $\{e_1, e_2, e_3\}$ be the corresponding orthonormal basis. The filament is free to deform in the half-space fluid domain $z \geq 0$, where $z = 0$ corresponds to a no-slip solid wall (see figure 1). The centerline of the filament is denoted by the position vector $\mathbf{r}(s, t)$, where $s$ and $t$ represent the arc-length and time, respectively. The balance of forces and moments on a cross section of the filament are given by Kirchhoff’s equations for an elastic rod

$$N' - f = 0, \quad M' + \hat{t} \times N = 0. \quad (1)$$

Here, the prime $(\cdot)' = \partial(\cdot)/\partial s$ denotes differentiation with respect to arc-length $s$, $\hat{t} = \mathbf{r}'/|\mathbf{r}'|$ is the tangent unit vector along the filament centerline, $\mathbf{N}$ and $\mathbf{M}$ are the internal force and bending moment, respectively, and $-\mathbf{f}$ is the drag force per unit length exerted by the surrounding fluid on the filament ($\mathbf{f}$ is the force per unit length exerted by the filament on the fluid). The Hookean constitutive relation between the bending moment $\mathbf{M}$ and the bending deformation (curvature) of the filament is given by $\mathbf{M} = B\hat{t} \times \hat{t}'$, where $B$ is the bending rigidity. The internal force $\mathbf{N}$ consists of a bending force and a constraint tension force that enforces the inextensibility condition.

The filament is free at its tip $s = \ell$ and is actuated by an internal motor at its base $s = 0$ that produces a torque $\mathbf{M}(0, t) = M_b \hat{e}_2$. The torque $M_b$ is a configuration-dependent torque that switches direction when the base angle $\theta_b(t)$ of the filament, defined as $\theta_b = \arcsin(e_3 \times \hat{t}(0, t) \cdot e_2)$, reaches predefined target orientations $\pm \Theta$. More specifically, we consider $M_b = \alpha M_b \hat{e}_2$, where $M_b$ is a positive constant and $\alpha \in \{-1, 1\}$ is a state variable that defines the torque direction; $\alpha$ changes from 1 to $-1$ at $\theta_b = \Theta$ and from $-1$ to 1 at
TABLE I. Characteristic scales of the system.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Dimensional value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Filament length</td>
<td>$\ell$</td>
<td>$20 , \mu m$</td>
</tr>
<tr>
<td>Fluid viscosity</td>
<td>$\mu$</td>
<td>$10^{-3} , \text{Pa} \cdot \text{s}$</td>
</tr>
<tr>
<td>Bending rigidity</td>
<td>$B$</td>
<td>$800 , \text{pN} \cdot \mu \text{m}^2$</td>
</tr>
<tr>
<td>Time scale</td>
<td>$T$</td>
<td>$\ell^4 \mu / B \cdot 0.2 , \text{s}$</td>
</tr>
</tbody>
</table>

$\theta_b = -\Theta$ (see figure 1). This torque model can be viewed as an extension to the geometric switch model for colloidal systems studied in\textsuperscript{6,24} and as a simplified version of the “geometric clutch” model proposed in\textsuperscript{28}. A target angle that acts as a geometric switch to drive elastic filaments along their entire length was used by\textsuperscript{7} to model the power and recovery strokes of eukaryotic cilia.

The fluid motion is governed by the incompressible Stokes equation for zero Reynolds number flows,

$$
-\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{F} = 0, \quad \nabla \cdot \mathbf{u} = 0.
$$

(2)

Here, $p$ is the pressure field, $\mu$ is the fluid viscosity, $\mathbf{u}$ is the fluid velocity field, and $\mathbf{F}$ is the (Eulerian) force density exerted by the filament on the fluid. $\mathbf{F}(\mathbf{x}, t)$ is related to the force per unit length $\mathbf{f}(s, t)$ as follows $\mathbf{F}(\mathbf{x}, t) = (1/A) \int_{s \in [0, \ell]} \mathbf{f}(s, t) \delta(\mathbf{x} - \mathbf{r}(s, t))\, ds$, where $A = \pi a^2 / 4$ is the cross-sectional area of the filament, assumed constant, $\delta$ is the three-dimensional Dirac $\delta$-function, and $\mathbf{x}$ is the position vector. These equations are subject to the no-slip condition $\mathbf{u} = 0$ at the bounding wall $z = 0$. We take advantage of the small aspect ratio $a/\ell \ll 1$ of the filament to approximate the velocity at the filament boundary by the velocity along its centerline,

$$
\mathbf{u}|_{\text{filament}} = \dot{\mathbf{r}}(s, t).
$$

(3)

To fully determine the filament deformation $\mathbf{r}(s, t)$ given the moment $\mathbf{M}_b$ at the filament base, we need to solve the coupled fluid-filament system of equations (1–3). It is convenient for building an efficient numerical method to (i) write the moment equation in (1) in integral form and (ii) assume that the filament is quasi-inextensible\textsuperscript{8,33,41}. In particular, we integrate the moment equation in (1) from the filament free end at $\ell$ to any location $s$ along the
filament, taking into account that \( M(\ell) = 0 \) and that along the filament \( N' = f \). We get, after an integration by parts on the second term, that

\[
M(s) + r \times \int_\ell^s f \, d\tilde{s} - \int_\ell^s r \times f \, d\tilde{s} = 0.
\]

We then write the force density \( f(s,t) \) applied by the filament on the surrounding fluid as \( f = f^\perp + f^\parallel \). We assume that the force component \( f^\parallel = (f \cdot \hat{t})\hat{t} \) tangent to the filament’s centerline can be obtained explicitly by considering a large tensile stiffness \( K \),

\[
f^\parallel = -K |r'| \hat{t},
\]

thus ensuring that the filament’s length remains almost constant. We substitute (5) into (4) taking into account that \( M = Br' \times r'' \) to obtain an expression for \( f^\perp \) in terms of the position vector \( r(s) \) and its spatial derivatives. To this end, one gets both components of the force density \( f = f^\perp + f^\parallel \) in terms of the kinematic variables \( r \) and its derivatives. We substitute these expressions for \( f \) into (2) and we solve numerically subject to (3) to obtain the nonlinear dynamics of the filament as discussed next.

To obtain non-dimensional counterparts to the equations of motion, we consider the dimensional scales associated with the fluid viscosity \( \mu \) and cilium length \( \ell \). Because of the geometric switch model, the system does not have an intrinsic time scale. To remedy this, we consider the time scale \( T = \ell^4 \mu / B \) arising from balancing the filament’s elasticity with the fluid viscosity. To this end, we consider the bending rigidity to be of the order \( B = 800 \text{ pN} \cdot \mu \text{m}^2 \), as reported in\(^47\) for wild type Chlamydomonas flagella. A list of the dimensional parameters used to scale the equations of the motion are reported in Table I. Hereafter, all quantities are considered to dimensionless unless otherwise stated.

III. NUMERICAL METHOD

We discretize the filament into a uniform chain of \( N + 1 \) segments of length \( a \) such that \( \Delta s = \ell / N = a \) (figure 1(b)). The segments are labeled from \( n = 0 \) at the filament base to \( n = N \) at its tip. The position vector is discretized by \( r_n = x_n e_1 + z_n e_3 \) and the local orientation \( \theta_n \) of the tangent vector to segment \( n \) is defined as the angle between the \( z \)-axis
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol Dimensionless value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of segments per filament</td>
<td>$N$</td>
</tr>
<tr>
<td>Segment length</td>
<td>$\Delta s = a$</td>
</tr>
<tr>
<td>Time step</td>
<td>$\Delta t$</td>
</tr>
<tr>
<td>Total integration time</td>
<td>$T$</td>
</tr>
<tr>
<td>Target angle</td>
<td>$\Theta$</td>
</tr>
<tr>
<td>Magnitude of base moment</td>
<td>$M_b$</td>
</tr>
<tr>
<td>Filaments separation distance</td>
<td>$d$</td>
</tr>
</tbody>
</table>

TABLE II. Dimensionless parameters used in simulations ($\ell, \mu$ and $B$ are normalized to 1).

and the vector $\Delta r_n = (r_{n+1} - r_n)$. Equation (4) can be written in discrete form as follows

$$M_{n-1} - \sum_{m \geq n}^N [(r_m - r_{n-1}) \times f_m] = 0.$$  \hspace{1cm} (6)

Here, $M_n = -B [(\theta_n - \theta_{n-1})/\Delta s] e_2$ for $1 \leq n < N$ whereas $M_o = M_b$ at the no-slip wall $z = 0$.

We decompose the force $f_n = f_n^\perp + f_n^\parallel$ exerted by segment $n$ on the surrounding fluid into two components $f_n^\perp$ and $f_n^\parallel$ that are perpendicular and parallel to $\Delta r_{n-1} = (r_n - r_{n-1})$. We substitute into (6) and rearrange the term containing $f_n^\perp$ to the other side of the equation to get

$$\Delta r_{n-1} \times f_n^\perp = M_{n-1} - \sum_{m > n}^N [(r_m - r_{n-1}) \times f_m].$$  \hspace{1cm} (7)

Upon taking the cross product with $\Delta r_{n-1}/\|\Delta r_{n-1}\|^2$, the above equation becomes

$$f_n^\perp = \left[ M_{n-1} - \sum_{m > n}^N (r_m - r_{n-1}) \times f_m \right] \times \frac{\Delta r_{n-1}}{\|\Delta r_{n-1}\|^2}.$$  \hspace{1cm} (8)

The parallel component $f_n^\parallel$ is given by the discrete analog to (5). Namely, for $1 \leq n < N$, one has

$$f_n^\parallel = -K \left[-\frac{\|\Delta r_n\| - \Delta s}{\Delta s} \frac{\Delta r_n}{\|\Delta r_n\|} \cdot \frac{\Delta r_{n-1}}{\|\Delta r_{n-1}\|} + \frac{\|\Delta r_{n-1}\| - \Delta s}{\Delta s} \frac{\Delta r_{n-1}}{\|\Delta r_{n-1}\|} \right] \frac{\Delta r_{n-1}}{\|\Delta r_{n-1}\|},$$  \hspace{1cm} (9)
FIG. 2. Filament dynamics for (a) $M_b = 1$ and (b) $M_b = 3$. From top to bottom: snapshots of the filament deformations, configuration-dependent moment $M_b$, angular velocity $\dot{\theta}_b$, angle $\theta_b$, and phase $\phi$ at the base of the filament as functions of time. Note that the frequency of oscillations is not known a priori, only the switching angles $\Theta = \pm 0.15\pi$.

whereas for $n = N$, one has

$$f^\parallel_N = -K\left(\frac{\Delta r_{N-1\parallel}}{\Delta s} - \Delta s\right) \frac{\Delta r_{N-1}}{\Delta s}$$

Using (8) and (9-10), $f_n$ can be evaluated sequentially from the filament tip (by decreasing order of $n$) in terms of the filament kinematic variables $r_m$, $m \geq n - 1$.

To solve (2-3), we use a one-dimensional distribution of regularized Stokeslets along the centerline of the filament together with an “image” distribution to impose the no-slip bound-
ary conditions at $z = 0$ plane. The regularized Stokeslets are placed at the center $r_n$ of each segment. The strength of the regularized Stokeslet at $r_n$ is equal to the discrete force $f_n$ and the fluid velocity generated by the filament at an arbitrary position $x$ in the fluid domain is given by $u(x) = \sum_{n=1}^{N} G(x - r_n) \cdot f_n$, where $G(x - r_n)$ is the Green's tensor for the regularized Stokeslet near a wall. We substitute this expression for the fluid velocity into (3), recalling (8) and (9-10) to express $f_n$ in terms of the filament position $r_m$. This yields a set of coupled equations for the filament dynamics that we evolve forward in time using the forward Euler method. Initial conditions for this system are the configuration of the filament $r(s, t)$ and the state variable $\alpha = \pm 1$.

In all numerical simulations, we fix the target angles at $\Theta = 0.15\pi$, we use $N = 20$ segments of length $a = 1/20$ to discretize the filament, and we set the regularization parameter of the Stokeslet to be equal to $a$. The tensile stiffness $K = 5000$ is a numerical parameter chosen to keep the length of the filament almost constant. The filaments are initialized in straight configuration normal to the wall. Here, the time step is $0.2 \times 10^{-4}$ and the system is integrated to $T = 20$, which is sufficient to capture the long-time dynamics; see Table II for a summary of all parameter values.

IV. DEFORMATION OF A SINGLE FILAMENT

We examine the motion of a single filament actively driven at its base by $M_b = \alpha M_b e_2$ ($\alpha = \pm 1$) that switches direction at $\Theta = \pm 0.15\pi$. Figure 2 shows the deformations and
FIG. 4. The filament with $M_b = 3$ recovers the same beating pattern when starting from a perturbed initial condition; the long-term beating pattern shown in green for comparison. (a) Filament with lower base moment converge to the long-term beating pattern within fewer cycles (see supplementary movies 1-4). (b) Filament with tilted angles produce asymmetric beating patterns. $M_b = 3$, target angles are $\pi/4 \pm \Theta$. Dashed line shows the average orientation $\pi/4$.

The frequency of switching in the drive is a property of the system that depends on the time evolution of the filament for two distinct values of the bending moment: (a) $M_b = 1$ and (b) $M_b = 3$. In each case, the moment $M_b$ is constant in magnitude between switches (figure 2, second row). In response, the angular velocity $\dot{\theta}_b$ slows down after each switching event (figure 2, third row). This decrease in $\dot{\theta}_b$ is induced by the internal restoring moment due to the filament elasticity, which acts in the opposite direction to $M_b$.

We introduce the phase variable $\phi \in [0, 1]$ as a linear interpolation of $\theta_b$ between the two target angles $\pm \Theta$,

$$\phi = \frac{\Theta + \alpha \theta_b}{4\Theta} + \frac{1 - \alpha}{4} = \begin{cases} \frac{\Theta + \theta_b}{4\Theta}, & \alpha = 1, \\ \frac{3\Theta - \theta_b}{4\Theta}, & \alpha = -1. \end{cases} \quad (11)$$

By definition, the values of $\phi$ lie in $[0, 0.5]$ when the base moment is positive ($\alpha = 1$) and $\phi \in [0.5, 1]$ when the base moment switches to negative ($\alpha = -1$). Thus, the phase variable $\phi$ is monotonic in time over one oscillation period (see figure 2, bottom row) and as a result, it can be viewed as a time re-parameterization for examining the long-term periodic behavior of the filament. We therefore label the snapshots in figure 2, top row, by their phase $\phi$.

The frequency of switching in the drive is a property of the system that depends on the
system’s parameters, including the magnitude of the base moment $M_b$. Figure 2 indicates that for $M_b = 1$, the base angle $\theta_b$ takes longer time to reach $\pm \Theta$ than for $M_b = 3$. To quantify the frequency $\omega$ of switching, we define it as the number of left-side switching events per unit time, averaged over late-time behavior. Figure 3 depicts $\omega$ as a function of $M_b$. The frequency $\omega$ increases monotonically with $M_b$ as well as the waviness of the filament. For $M_b$ larger than 1.7, the curvature along the filament $(0 < s < \ell)$ changes sign at least once, indicating a clear traveling-wave pattern. The switching frequency can be mapped to a Sperm number $Sp = ( / \xi / B)^{1/4}$, defined as the ratio between the filament length and the elasto-viscous penetration length. Here, $\xi = 4\pi \mu / \ln(2\ell/a)$ is the local drag coefficient perpendicular to the filament direction. The Sperm number $Sp$ increases monotonically with $M_b$, ranging from 1.6 to 4.3 for $M_b \in [0.5, 3]$. This range of Sperm numbers is consistent with those observed empirically in flagella and cilia. For example, the wild type *Chlamydomonas* has a beating frequency of 60-80 Hz, which yields a Sperm number $Sp \approx 3$, given the characteristic parameters listed in Table I.

To conclude this section, we note that the long-term behavior of the filament depends on $M_b$ but it is independent of the filament initial configuration, as illustrated in figure 4(a). Also, we note that so far the filament deformations are symmetric because the switching orientations $\pm \Theta$ are equal and opposite. To break this symmetry, it suffices to tilt the angle about which the geometric switch is applied by setting $\Theta_{\text{left}} = \Theta_{\text{right}}$ as shown in figure 4(b). Hereafter, we restrict our discussion to the symmetric case.

V. SYNCHRONIZATION OF TWO FILAMENTS

We consider the behavior of two hydrodynamically-coupled, elastic filaments separated by a distance $d$ and subject to the same moment $M_b$ at their base. We set the separation distance to be large enough ($d > 0.4$) so that the two filaments do not intersect.

Figure 5 shows the long-term behavior of two filaments that start in a nearly anti-phase configuration; the left filament, referred to as filament 1, is initially straight and moving to the right ($\alpha_1(0) = 1$) whereas the right filament, or filament 2, is initially moving to the left ($\alpha_2(0) = -1$) such that the phase difference is equal to $\Delta \phi(0) = \phi_2(0) - \phi_1(0) = 0.49$. Here, the state variables $\alpha_1$ and $\alpha_2$ and phase variables $\phi_1$ and $\phi_2$ for filaments 1 and 2 are defined as in (11). This initial configuration corresponds to a small perturbation away from
FIG. 5. Long term dynamics of a pair of filaments with (a) $M_b = 1$ and (b) $M_b = 3$ for $d = 0.7$ and $\Delta \phi(0) = 0.49$. Top: beating patterns at four different phases ($\phi_1 = 0, 0.25, 0.5, 0.75$). Middle: base angles $\theta_b$ as a function of time for $0 < t < 0.3$ (to highlight transient behavior). Bottom: phase difference $|\Delta \phi|$ for $0 < t < 2$.

the anti-phase configuration for which $\Delta \phi = 0.5$. The coupling between the two filaments is due to hydrodynamic interactions only.

The two filaments exhibit anti-phase synchronization for $M_b = 1$ and $d = 0.7$ as shown in 5(a), whereas for $M_b = 3$ the two filaments depart from their anti-phase initial conditions and approach in-phase synchronization as shown in Figure 5(b). These modes of synchronization are quantified in Figure 5(c). In both cases, the shapes of the filaments show no significant difference compared to those exhibited by the single filaments.

To quantify the long-term synchronization mode between the two filaments, we adapt the synchronization order parameter $Q$ proposed in\textsuperscript{24}. Namely, we let

$$Q = \frac{-1}{T - T^*} \int_{T^*}^{T} \alpha_1(t) \alpha_2(t) dt,$$

where $T$ is the total integration time, $T^*$ is chosen to ensure that transient behavior is excluded. By construction, one has $-1 \leq Q \leq 1$, where $Q = -1$ describes exactly in-phase motions while $Q = 1$ corresponds to exactly anti-phase motions. In the simulations, we
FIG. 6. Synchronization order parameter $Q$ as a function of bending moment $M_b$ (Panels (a) and (b)), and as a function of separation distance $d$ (Panels (c) and (d)). (a) and (c) In-phase initial conditions are shown in blue and anti-phase in red. (b) and (d) Mean $\langle Q \rangle$ (dotted line) and standard deviation $\text{SD}(Q)$ (grey error bars) corresponding to 20 random initial conditions; $Q$ values are shown as blue and red dots, with color intensity proportional to the percentage of initial conditions resulting in these values.

set $T^* = 15$ and $T = 20$ time units, respectively; the filaments are said to be in-phase if $Q \in [-1, -0.5]$ and anti-phase if $Q \in [0.5, 1]$.

We fix the separation distance between the filaments at $d = 0.7$ and investigate the effect of the bending moment $M_b$ on the long-term synchronization modes between the two filaments. We consider in-phase and anti-phase initial conditions $\Delta \phi(0) = 0$ and $\Delta \phi(0) = 0.5$, respectively, as well as small perturbations $\Delta \phi(0) = 0.01$ and $\Delta \phi(0) = 0.49$ away from these configurations. Figure 6(a) depicts the synchronization order parameter $Q$ versus $M_b$ shown in blue for $\Delta \phi(0) = 0$ and $\Delta \phi(0) = 0.01$ and in red for $\Delta \phi(0) = 0.5$ and $\Delta \phi(0) = 0.49$. When starting at $\Delta \phi = 0.5$, the filaments always synchronize anti-phase. However, this anti-phase synchronization become unstable for large $M_b$ (dashed red line) because the filaments shift to in-phase synchronization under a small perturbation in the initial conditions ($\Delta \phi(0) = 0.49$). On the other hand, when starting at $\Delta \phi = 0$ and $\Delta \phi =$
FIG. 7. Beating frequency $\omega$ as a function of bending moment $M_b$ (Panels (a) and (b)), and as a function of separation distance $d$ (Panels (c) and (d)). (a) and (c) In-phase initial conditions are shown in blue and anti-phase in red. (b) and (d) Mean $\langle \omega \rangle$ (dotted line) and standard deviation SD($\omega$) (grey error bars) corresponding to 20 random initial conditions; $\omega$ values are shown as blue and red dots, with color intensity proportional to the percentage of initial conditions resulting in these values. In all panels, the frequency of a single filament (dashed black line) is superimposed for comparison.

For $M_b \leq 0.01$, the filament synchronize in-phase for small $M_b$, shift to anti-phase synchronization as $M_b$ increases, and shift back to in-phase synchronization as $M_b$ increases further. For $0.6 \leq M_b \leq 0.9$ and $2.1 \leq M_b \leq 2.4$, the filaments exhibit both stable in-phase and stable anti-phase synchronization depending on initial conditions. To better understand the sensitivity of these synchronization modes to perturbations in the initial conditions, we perform Monte Carlo simulations with initial conditions randomly chosen from a uniform distribution function $\Delta \phi(0) \in U(-0.5, 0.5)$. Statistical results of the synchronization modes based on 20 Monte Carlo simulations are shown in figure 6(b). Dotted lines and error bars depict the mean $\langle Q \rangle$ and standard deviation SD($Q$) of the synchronization order parameter respectively. Overlaid blue and red dots are the distributions of the Monte Carlo simulations, colored in blue and red according to the emergent synchronization modes (blue for in-
phase and vice-versa. The color intensity of the dots represents the fraction of simulations corresponding to a particular $Q$ value – lighter color means fewer simulations out of 20 total number of simulations. The bistable regions where both red and blue dots co-exist are consistent with the results in figure 6(a). In the bistable regions, the synchronization mode is sensitive to initial conditions.

To explore the effect of the separation distance $d$ between the filaments on the emergent synchronization modes, we fix the magnitude of the bending moment at $M_b = 2$ and plot the synchronization order parameter $Q$ versus $d$ in figure 6(c,d). For small $d$, all initial conditions lead to anti-phase synchronization. As $d$ increases, both in-phase and anti-phase synchronizations co-exist, depending on initial conditions, and as $d$ increases further, only in-phase synchronization are observed. The Monte Carlo simulations shown in figure 6(d) are consistent with these findings. In the limit $d \to \infty$, the two filaments maintain their initial phase difference. In other words, as $d \to \infty$, the two filaments will take infinitely long time to synchronize.

In Figure 7, we report the values of the emergent beating frequencies for the cases considered in figure 6 and compare these values to the case of a single filament from figure 3, which we show in black dashed lines in figure 7. The beating frequencies for the pair of filaments are either faster or slower than the single filament depending on their synchronization modes: anti-phase filaments beat at lower frequencies because the two filaments “work against each other” while in-phase filaments beat at higher frequencies because they “work together”. In particular, in anti-phase beating the two fibers are compressing and extending fluid elements in the region between them while for in-phase beating, the fluid and the filaments move together. In the limit $d \to \infty$, the beating frequency for the pair of filaments converges to the beating frequency of a single filament.

Figure 8 shows the synchronization order parameter $Q$ over the parameter space $(d, M_b)$; figure 8(a) shows $Q$ for nearly in-phase initial conditions $\Delta \phi(0) = 0.01$ and figure 8(b) for nearly anti-phase initial conditions $\Delta \phi = 0.49$. Figures 8(c,d) show the mean and standard deviation, respectively, of $Q$ for 20 Monte Carlo simulations with initial phase differences chosen from a uniform distribution $\mathcal{U}(-0.5, 0.5)$. Taken together, these results imply that the parameter space can be divided into three distinct regions: a stable anti-phase region where $\langle Q \rangle \in [0.5, 1]$ and $\text{SD}(Q) < 0.2$; a stable in-phase region where $\langle Q \rangle \in [-1, -0.5]$ and $\text{SD}(Q) < 0.2$; and a bistable region where $\langle Q \rangle \in [-0.5, 0.5]$ and $\text{SD}(Q) > 0.2$, in which the
FIG. 8. Synchronization order parameter of two filaments as a function of bending moment $M_b$ and separation distance $d$ for (a) nearly in-phase ($\Delta \phi(0) = 0.01$), (b) nearly anti-phase ($\Delta \phi(0) = 0.49$), and (c) and (d) 20 randomly chosen initial conditions. $\langle Q \rangle$ and $\text{SD}(Q)$ are the mean and standard deviation of synchronization order parameter. High $\text{SD}(Q)$ indicates sensitivity to initial conditions. (e) In-phase, anti-phase and bistable regions obtained by overlaying (c) and (d).

synchronization states are sensitive to the initial phase differences. The three regions are illustrated in figure 8(e).

VI. SHAPE-DEPENDENT OSCILLATORS

In the geometric-switch model proposed by^{24} and^{6}, a rigid spherical particle is free to move along one-direction, say the $x$-axis, under the influence of a driving force $F$ that switches direction when the particle position reaches predefined target positions. Here, we develop a phenomenological model, based on the geometric switch oscillator, that accounts for the filament’s elasticity and shape changes in terms of a “lumped” shape variable, which we denote by $s$ (not to be confused with the filament’s arclength $s$); see figure 1(c). We propose the coupled position-shape system of equations

$$\xi(s) \dot{x} = -ks + \alpha F,$$

$$\tau \dot{s} = -s + \alpha F. \tag{13}$$
The elastic “particle” is subject to a configuration-dependent force $\alpha F$, where the magnitude $F$ is constant whereas $\alpha$ switches between $\{-1, 1\}$ as the particle position reaches a predefined oscillation amplitude $|x| = X_s$. For a rigid particle, the drive $F$ is balanced by a hydrodynamic drag equal to $\xi \dot{x}$, where $\xi$ is a constant (positive) drag coefficient. Elasticity introduces an internal restoring force that competes with the driving force and couples the shape $s$ to the orientation dynamics. The elastic force is modeled via a spring with stiffness coefficient $k$ that represents a “lumped” elastic modulus of the filament. The drag coefficient $\xi$ also depends on shape; it should be maximum when $s = 0$, that is, when the filament is straight and moving transversally to itself, and minimum when the filament reaches its maximum deformation. It should also be symmetric under reflections from $s$ to $-s$. We therefore set $\xi(s) = \max(\xi_o - bs^2, \epsilon)$, where the quadratic function $\xi_o - bs^2$ is maximum at and symmetric about $s = 0$ and the parameter $b$ characterizes the dependence of $\xi$ on shape. The lower bound $\epsilon > 0$ ensures that the drag coefficient $\xi$ remains positive at all time.

The shape of the filament changes under the influence of the driving force but relaxes to its original shape when it is not actuated. In (13), we assume that $\alpha F$ drives the shape directly and that the shape $s$ relaxes to the original shape $s_o$ with constant relaxation parameter $\tau$. For a fixed value of $\alpha$, the solution to the shape equation is of the form $s = \alpha F + (s_o - \alpha F)e^{-t/\tau}$, where $s$ relaxes to $s_o$ when $F = 0$. For non-zero $F$, the force switches sign at $\pm X_s$, thus coupling position and shape. An alternative form of the shape equation in (13) could be written by using $\dot{x}$ in the shape equation instead of directly driving it by $\alpha F$. Then, the shape equation becomes nonlinear. We chose the linear form in (13) because we are mainly interested in reducing the complexity of the dynamical system, while identifying the main physical mechanisms at play.

Figure 9(a) shows the typical evolution of $\dot{x}$ for the shape-dependent oscillator. The dynamics resembles qualitatively the dynamics of the full filament model shown in the second row of figure 2. Specifically, after each switch, the velocity $\dot{x}$ first experiences a sharp decrease and remains small until the next switch. This is a joint effect of the internal restoring moment $-ks$ due to the filament elasticity and the shape-dependent drag coefficient $\xi(s)$. If the restoring moment is eliminated ($k = 0$), the velocity profile changes such that it first decreases then increases (figure 9(b)), and if the drag coefficient is held constant ($b = 0$), the decrease in velocity after each switch is more gradual (figure 9(c)). In the case of the standard geometric switch $b = k = 0$, the velocity remains constant after each switch.
FIG. 9. Velocity evolution $\dot{x}$ versus time $t$ of the single shape-dependent oscillator for: (a) Shape-dependent oscillator, $b = 0.5$, $k = 0.5$; (b) no restoring force, $b = 0.5$, $k = 0$; (c) constant drag coefficient, $b = 0$, $k = 0.5$; and (d) traditional oscillator, $b = 0$, $k = 0$. In all cases, $\tau = 1$, $\xi_o = 1$, $X_s = 1$, $F = 1$.

because the applied force considered here is constant (figure 9(d)).

We now consider two hydrodynamically-coupled, shape-dependent oscillators,

$$\xi(s_i)[\dot{x}_i - v_j(x_i)] = -ks_i + \alpha_iF,$$

$$\tau s_i = -s_i + \alpha_iF. \tag{14}$$

Subscripts $i, j = 1, 2$ are the oscillator indices and $v_j(\theta_i) = \dot{x}_j/|x_i - x_j|$ (with $i \neq j$) is the far-field approximation of the flow velocity generated by the motion of oscillator $j$ at $x_i$. The state variable $\alpha_1$ switches between $\{-1, 1\}$ once $|x_1| = X_s$, while $\alpha_2$ switches between $\{-1, 1\}$ once $|x_2 - d| = X_s$, where $d$ is the separation distance between the centers of the two oscillator trajectories.

If $b = k = 0$, the first equation in (14) is consistent with the geometric switch oscillators in$^{6,24}$ with one major distinction: here the applied force has constant magnitude. In their model, the applied force depends on the particle position, which determines the type of synchronization: the two oscillators synchronize anti-phase if the force magnitude decreases as the oscillator approaches $X_s$ and in-phase if the force magnitude increases. For constant force, the two oscillators do not synchronize. Nowhere bistable synchronizations are observed. Consistent with their findings, when the shape changes are not accounted for ($b = k = 0$), the model in (14) exhibits no synchronization – the two oscillators maintain their initial phase difference for all time. However, when shape changes are considered ($b \neq 0$
FIG. 10. Synchronization modes of two shape dependent oscillators as a function of applied force $F$ and separation distance $d$ for (a) nearly in-phase ($\Delta \phi(0) = 0.01$), (b) nearly anti-phase ($\Delta \phi(0) = 0.49$), and (c) and (d) 20 randomly chosen initial conditions. $\langle Q \rangle$ and $\text{SD}(Q)$ are the mean and standard deviation of synchronization order parameter. High $\text{SD}(Q)$ indicates sensitivity to initial conditions. (e) In-phase, anti-phase and bistable regions obtained by overlaying (c) and (d). In all simulations, $\tau = 1$, $b = 2$, $k = 0.1$, $X_S = 1$, $\xi_o = 1$, and $k \neq 0$), multiple synchronization modes can arise depending on the parameter values and initial conditions as shown in figure 10.

Figures 10(a) and (b) show the synchronization order parameter $Q$ as a function of the force magnitude $F$ and separation distance $d$ for two sets of initial conditions $\Delta \phi(0) = 0.01$ and $\Delta \phi(0) = 0.49$, respectively. For both initial conditions, in-phase synchronization is favored as $F$ increases, albeit for different values of $F$. This tendency to synchronize in-phase at larger $F$ is consistent with the trend observed in the full filament model. Figures 10(c) and (d) show the results of 20 Monte Carlo simulations with random initial conditions taken from a uniform distribution function: a stable anti-phase region is observed for $F < 0.3$, a stable in-phase region for $F > 0.7$, and a bistable region for $0.3 < F < 0.7$. The three regions are illustrated in figure 10(e).

The simple model in (14) captures some of the main features of the full filament model. In particular, it shows the presence of regions where in-phase and anti-phase oscillations are both stable, depending on initial conditions. This bistability is the product of the coupling between hydrodynamic interactions and shape changes. In fact, if the restoring force due to elasticity is eliminated ($k = 0$ but $b > 0$), the oscillators always synchronize in phase.
Meanwhile, if the dependence of drag on shape is eliminated \((b = 0 \text{ but } k > 0)\), the oscillators always synchronize anti-phase. The two types of synchronization modes are observed only when the two effects of \(k\) and \(b\) are present. These findings imply that the two different synchronization modes observed in the simplified shape-dependent oscillators and in the full filament model are due to the interplay between elasticity, shape-dependent drag, and hydrodynamic coupling.

VII. DISCUSSION

The main contributions of this work can be summarized as follows:

(i) We proposed a model for elastic micro-filaments of finite length submerged in viscous fluid; the filaments are attached to a wall and driven at their base by a bending moment that is geometrically-triggered to switch direction as the filament approaches pre-defined target angles. This filament model, although not biologically accurate, carries many features that are common to biological flagella and cilia such as form compliance and maximum driving moments at or close to the base.

(ii) Full hydrodynamic interactions among and within filaments were considered, and the resulting equations were solved numerically. Single filaments were shown to undergo long-term periodic deformations that are insensitive to initial conditions and whose waviness and frequency increased with increasing the intensity of the driving moment. It is worth noting that throughout this study, we fixed the bending rigidity of the filament and changed the intensity of the drive. This is equivalent to fixing the magnitude of the drive and varying the filament compliance.

(iii) Pairs of filaments exhibit stable in-phase and anti-phase synchrony that are robust to initial perturbations; more interestingly, both in-phase and anti-phase synchronizations stably co-exist in regions of the parameter space (driving moment versus separation distance), with in-phase synchrony associated with higher oscillation frequencies. These multiple synchronization modes are inherently non-linear and cannot be captured in a linear stability analysis.

(iv) To explain the main mechanisms underlying the observed behavior, we proposed a low-order model of an elastic “particle” that accounts for shape changes in terms of a
“lumped” shape variable that is coupled to the particle’s position. The simpler model recapitulates the behavior observed in single and pair of filaments and highlights the role of each component – elasticity, shape-dependent drag, and hydrodynamic coupling – in the emergent behavior.

(v) Our low-order model is consistent with the geometric switch oscillators of\(^6,24\). In the latter, the driving force depends on the particle configuration, and its functional form determines the type of synchronization: two oscillators synchronize anti-phase if the force magnitude decreases as each oscillator approaches its switching positions and in-phase if the force magnitude increases. Shifting between different synchronization modes requires changing the model of the driving force. In contrast, in our models, the magnitude of the drive is independent of configuration. Stable in-phase or anti-phase as well as bistable synchronization modes, all arise without the need to change the functional form of the drive. A transition from in-phase to anti-phase synchrony can be induced by varying the drive level or at the same drive level by perturbing the initial conditions. On a more abstract level, the dynamics in our models can be thought of as associated with one potential landscape with multiple local minima that can be visited by either changing the parameter values or the initial conditions.

These findings – namely, the co-existence of in-phase and anti-phase synchrony and the fact that in-phase synchrony is associated with higher frequencies and filament waviness (traveling-wave deformations) – are consistent with experimental observations in a *Chlamydomonas* biflagellate\(^{27}\). Flagella were shown to switch stochastically between anti-phase and in-phase states, and that the latter has a distinct waveform and significantly higher frequency (the notation in-phase and anti-phase is reversed in\(^{27}\)). In the context of our model, such switching could occur due to random perturbations or by varying the intensity of the internal drive. This is in contrast to alternating between different models of the drive characterized by different modes of synchrony\(^{27}\). The distinction between these two views – keeping the same form of the drive or alternating between different drive forms – is fundamentally linked to admissible hypotheses on the physiological and biophysical mechanisms underlying the transition between different synchronization modes. For example, in light of our results, it is plausible that transitions in biflagellar synchrony are triggered purely mechanically, say by random noise in the medium, without biochemical changes that alter
the driving forces, or physiologically by modifying either the intensity of the drive or the 
compliance of the flagella, without inducing new behavior in the internal machinery.

Models similar to the one presented here could thus serve to guide future research and 
formulate new hypotheses regarding the mechanisms that drive and alter synchrony in bio-
logical and physical systems. Future extensions of this work will account for more accurate 
models of the internal driving moments\textsuperscript{14,39}, three-dimensional filament deformations with 
torsion and twist\textsuperscript{29,34}, and multiple interacting filaments with application to metachronal 
coordination of cilia\textsuperscript{19,21,22,31,48}.

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