A new basis for filament simulation in three dimensions

Benjamin J. Walker,† Kenta Ishimoto,‡ and Eamonn A. Gaffney†

†Wolfson Centre for Mathematical Biology, Mathematical Institute, University of Oxford, Oxford, OX2 6GG, UK
‡Graduate School of Mathematical Sciences, The University of Tokyo, Tokyo, 153-8914, Japan

(Dated: July 5, 2019)

Simulations of slender inextensible filaments in a viscous fluid are often plagued by numerical stiffness. Recent coarse-graining studies have reduced the computational requirements of such systems, though have thus far been limited to the motion of planar filaments. In this work we extend such frameworks to filament motion in three dimensions, identifying and circumventing artificial singularities introduced by filament parameterisation via repeated changes of basis. The resulting methodology enables efficient and rapid study of the motion of flexible filaments in three dimensions, and is readily extensible to a wide range of problems, including filament motion in confined geometries, large-scale active matter simulations, and the motility of mammalian spermatozoa.

PACS numbers: 47.15.G-, 47.63.Gd, 87.15.La

INTRODUCTION

The coupled elastohydrodynamics of flexible filaments on the microscale are of significance to much of biology [1,3], in addition to being of pertinence to the development of microdevices and interaction of flows near surfaces [4,5]. The complex mechanics of fluid-structure interaction has been well studied, as illustrated by the slender body theory of Tornberg and Shelley [6] and Liu et al. [7] and the boundary element computations of Pozrikidis [8]. Necessary to the numerical study of filament mechanics is an appropriate framework, capable of realising efficient simulation of coupled filament elastohydrodynamics, as noted in the recent extensive review of du Roure et al. [9]. To this end, in this work we develop and implement a framework for the solution of the elastohydrodynamics of an inextensible, unshearable filament in three spatial dimensions, attempting to circumvent the extreme numerical stiffness typically associated with the mechanics of filaments in a viscous fluid. Recent developments in this field include the work of Schoeller et al. [10], which utilises a quaternion representation of filament orientation to parameterise the three dimensional shape of the slender body and makes use of the force coupling method [11]. In the framework of Schoeller et al. [10] significant numerical care is required to satisfy the condition of filament inextensibility, thus there is scope for the development of an accurate modelling framework that circumvents the computational work typically needed to satisfy this constraint.

A core motivation for developing this framework is the mechanics of filaments used to drive cellular swimming, for example the sperm flagellum. This readily exhibits three dimensional motions, and previous studies of the fluid-structure coupling between sperm-flagella and the surrounding fluid have been plagued by extreme numerical stiffness, to the extent that practical simulation studies have been limited and parameter space studies are all but prohibitive [12,13]. Hence, our fundamental objective is to develop a simulation framework for studying the mechanics of a general twistable rod that can bend in any direction. Further, we aim to present such a framework that also circumvents the extreme numerical stiffness of earlier developments to enable the study of large parameter spaces and collective behaviour in the physics of swimming cells, and in turn cellular active matter.

In this study we will seek to extend the recent work of Moreau et al. [14], Walker et al. [15], Hall-McNair et al. [16] to three dimensions, attempting to retain the reduction in numerical stiffness offered by their methodologies. We aim to cast the elastohydrodynamical problem in such a way as to be readily solvable by existing numerical methods, and further such that it is extensible to a variety of modelling problems, from clamped filaments in flow as studied by Pozrikidis [8], Walker et al. [15] to the collective motion of active filaments.

METHODS

Equations of elasticity

We consider a slender inextensible unshearable filament in a viscous Newtonian fluid with centreline described by \( \mathbf{x}(s) \), parameterised by arclength \( s \in [0,L] \) for filament length \( L \). Here and throughout, the Reynolds number will be taken to be identically zero. Along the filament we have the pointwise conditions of force and moment balance, given explicitly by

\[
\mathbf{n}_s - \mathbf{f} = 0, \tag{1}
\]

\[
\mathbf{m}_s + \mathbf{x}_s \times \mathbf{n} - \tau = 0, \tag{2}
\]

for contact force and couple denoted \( \mathbf{n}, \mathbf{m} \) respectively and where a subscript of \( s \) denotes differentiation with respect to arclength. The quantity \( \mathbf{f} \) is the force per unit
length applied on the fluid medium by the filament, which we will later express in terms of the filament velocity $\dot{x}$, where here dot denotes a time derivative. Similarly, $\tau$ is the torque per unit length applied on the fluid medium by the rotation of the filament. Following the approach of Moreau et al. [14], integrating these pointwise balance equations under the assumptions of zero contact force and couple at the tip of the filament yields the integrated balance equations

$$- \int_0^L f(s) \, ds = n(0),$$

$$- \int_0^L [(x(\delta) - x(s)) \times f(\delta) + \tau(\delta)] \, d\delta = m(s).$$

Given a right-handed orthonormal basis \( \{d_1(s), d_2(s), d_3(s)\} \) such that \( d_3 \) corresponds to the local filament tangent, following the approach of Nizette and Goriely [17] for \( \alpha = 1, 2, 3 \) we define the twist vector \( \kappa \) by

$$\frac{\partial d_\alpha}{\partial s} = \kappa \times d_\alpha.$$

Writing \( \kappa = \sum_\alpha \kappa_\alpha d_\alpha \), for bending stiffness \( EI \) we adopt a linear constitutive relation between the torques \( m \) and the twist vector \( \kappa \), written explicitly as

$$m = EI \left( \kappa_1 d_1 + \kappa_2 d_2 + \frac{1}{1 + \sigma} \kappa_3 d_3 \right),$$

where \( \sigma \) is the Poisson ratio [17]. With this constitutive relation the integrated moment balance equations in the \( d_\alpha \) directions are simply

$$- d_\alpha(s) \cdot \int_0^L [(x(\delta) - x(s)) \times f(\delta) + \tau(\delta)] \, d\delta = \frac{EI}{1 + \delta_{\alpha,3}\sigma} \kappa_\alpha(s),$$

for \( \alpha = 1, 2, 3 \) and where \( \delta_{\alpha,\beta} \) denotes the Kronecker delta.

**Filament discretisation**

In discretising the filament we follow the approach of Walker et al. [13], as previously applied to planar filaments and itself building upon the earlier work of Moreau et al. [14]. We approximate the filament with \( N \) piecewise-linear segments, each of constant length \( \Delta s \), with segment endpoints having positions denoted by \( x_1, \ldots, x_{N+1} \) and the inextensibility constraint satisfied inherently. The endpoints of the \( i \)th segment correspond to \( x_i \) and \( x_{i+1} \) for \( i = 1, \ldots, N \), with the local tangent \( d_3 \) being constant on each segment and denoted \( d_3^i \). In what follows we will consider a choice of \( d_1^i, d_2^i \) such that they are also constant on each segment, without loss of generality, and we denote these constants similarly as \( d_1^1, d_2^1 \). Writing \( s_i \) for the constant arclength associated with each material point \( x_i \), we apply Eq. (7) at each of the \( s_i \) for \( i = 1, \ldots, N \), splitting the integral at the segment endpoints to give

$$- d_\alpha^i \cdot \sum_{j=1}^{N} (s_{j+1}) \int_0^L [(x(\delta) - x_i) \times f(\delta) + \tau(\delta)] \, d\delta = \frac{EI}{1 + \delta_{\alpha,3}\sigma} \kappa_\alpha(s_i),$$

for \( \alpha = 1, 2, 3 \). On the \( j \)th segment, \( x \) may be written as \( x(s) = x_j + \eta(x_{j+1} - x_j) \), where \( \eta \in [0,1] \) is given by \( \eta = (s - s_j)/\Delta s \). Additionally, discretising the force per unit length as a continuous piecewise-linear function, with \( \eta \) as above we have \( f(s) = f_j + \eta(f_{j+1} - f_j) \) on the segment, where we write \( f_j = f(s_j) \). Substitution of these parameterisations into Eq. (8) and subsequent integration yields, after simplification,

$$- d_\alpha^i \cdot (I_i^f + I_i^\tau) = \frac{EI}{1 + \delta_{\alpha,3}\sigma} \kappa_\alpha(s_i),$$

where the integral contribution of the force and torque densities are denoted \( I_i^f \) and \( I_i^\tau \) respectively. With this discretisation \( I_i^f \) has reduced to

$$\sum_{j=1}^{N} \left\{ \left[ \frac{\Delta s}{2} (x_j - x_i) + \frac{\Delta s^2}{6} d_3^i \right] \times f_j + \left[ \frac{\Delta s}{2} (x_j - x_i) + \frac{\Delta s^2}{3} d_3^i \right] \times f_{j+1} \right\}.$$

For \( I_i^\tau \) we consider a piecewise constant discretisation of the torque per unit length, taking \( \tau = \tau_j \) on the \( j \)th segment. This yields the simple expression

$$I_i^\tau = \sum_{j=1}^{N} \Delta s \tau_j.$$

From the above we see explicitly that the integral component of each moment balance equation may be written as a linear operator on the \( f_j \) and the \( \tau_j \), noting that the cyclic property of the scalar triple product further simplifies the vector products in the above representation.

Similarly, with this piecewise-linear discretisation the integrated force balance of Eq. (3) simply reads

$$- \frac{\Delta s}{2} \sum_{j=1}^{N} (f_j + f_{j+1}) = n(0).$$
We write $F = [f_{1x}, f_{1y}, f_{1z}, \ldots, f_{N+1,x}, f_{N+1,y}, f_{N+1,z}]^\top$ for components $f_{jx, y, f_{jz}}$ of $f_j$ with respect to some fixed laboratory frame with basis $\{e_x, e_y, e_z\}$, and similarly $T$ for the vector of components of torque per unit length. With this notation we may write the equations of force and moment balance as
\begin{align}
-\mathcal{B} \begin{bmatrix} F \\ T \end{bmatrix} = R, \tag{13}
\end{align}
where $\mathcal{B}$ is a matrix of dimension $(3N + 3) \times (6N + 3)$ with rows $B_i$. For $k = 1, 2, 3$ these are given by
\begin{align}
B_1 &= \frac{\Delta s}{2} \begin{bmatrix} 1, 0, 0, 2, 0, 0, 2, 0, 0, 1, 0, 0 \end{bmatrix}, \\
B_2 &= \frac{\Delta s}{2} \begin{bmatrix} 0, 1, 0, 0, 2, 0, 0, 2, 0, 0, 1, 0 \end{bmatrix}, \\
B_3 &= \frac{\Delta s}{2} \begin{bmatrix} 0, 0, 1, 0, 0, 2, 0, 0, 2, 0, 0, 1 \end{bmatrix}, \tag{14}
\end{align}
and correspond to the force balance equation Eq. (12). The remaining rows of $\mathcal{B}$ encode the moment balance equation. Accordingly, and under the assumption of a force-free filament base, the $(3N + 3)$-vector $R$ is given by
\begin{align}
R = \frac{EI}{1 + \delta_{\alpha,3\sigma}} \begin{bmatrix} E_1(s_j), E_2(s_j), E_3(s_j) \end{bmatrix} \text{ } j = 1, \ldots, N \tag{15}
\end{align}
We remark that each of the quantities involved in the construction of $B$ and $R$ are well-defined for a general filament in three dimensions, subject to a choice of $d_1$ and $d_2$ and computing the components of the twist vector as $\kappa_1 = d_3 \cdot \partial_x d_2$, $\kappa_2 = d_1 \cdot \partial_x d_3$, and $\kappa_3 = d_2 \cdot \partial_x d_1$. Additionally, we will proceed assuming that the filament is moment-free at the base, which additionally enforces $\kappa_1(0) = \kappa_2(0) = \kappa_3(0) = 0$.

**Coupling hydrodynamics**

We now relate the force density $f$ acting on the fluid to the velocity of each segment endpoint, utilising the commonly-applied method of resistive force theory as introduced by Hancock [13], Gray and Hancock [19] and adopted by Moreau et al. [14] for planar filaments. Here taking the radius of the filament to be $\epsilon = 10^{-2} L$, simple resistive force theory gives the leading order relation between filament velocity and force density as
\begin{align}
f_t = -C_t u_t, \quad f_n = -C_n u_n. \tag{16}
\end{align}
Here $f_t$ and $f_n$ denote the components of the force density tangential and normal to the filament, with analogous definitions of $u_t$ and $u_n$, and the resistive coefficients $C_t$ and $C_n$ are related by $C_n = 2C_t$. We will utilise the expression of Gray and Hancock [19], with
\begin{align}
C_t = \frac{2\pi \mu}{\log(2/\epsilon) - 0.5}, \quad C_n = \frac{4\pi \mu}{\log(2/\epsilon) - 0.5}. \tag{17}
\end{align}
We approximate the local filament tangent at the endpoint $x_i$ as the average of $d_3^{-1}$ and $d_3^0$ for $i = 2, \ldots, N$, with the tangent for $i = 1$ and $i = N + 1$ simply being taken as $d_3^1$ and $d_3^N$ respectively. By linearity, and again assuming a piecewise-linear force density along segments, we may write the coupling of kinematics to hydrodynamics as
\begin{align}
\dot{X} = A F, \tag{18}
\end{align}
where $A$ is a square matrix of dimension $3(N + 1) \times 3(N + 1)$ and is a function only of the segment endpoints $x_i$. Of dimension $3(N + 1)$, the vector $X$ corresponds to the velocities of the segment endpoints, and is constructed analogously to $F$ with respect to the laboratory frame. This relation results from the application of the no-slip condition at the segment endpoints, coupling the filament to the surrounding fluid.

In order to relate the rate of rotation of each segment to the viscous torque $\tau_i$ acting on it, we here consider an approximation of the finite segment as an infinite rotating cylinder, associating the torque per unit length on the $i$th segment with the rotation $\omega_i$ about its local tangent $d_3^i$ via the relation of Chwang and Wu [20]:
\begin{align}
\tau_i = 4\pi \mu e^2 \omega_i d_3^i. \tag{19}
\end{align}
Here $\mu$ is the viscosity of the fluid medium, and we recall that $\epsilon$ is the radius of the filament. We may write this relation as a linear operator on $\omega = [\omega_1, \ldots, \omega_N]^\top$, written simply as $T = \hat{A} \omega$. This crude approximation may readily be substituted for non-local hydrodynamics via the method of regularised Stokeslet segments, which will likely be a topic of future work. Similarly, non-local hydrodynamics may be utilised in place of Eq. (18), as used for two-dimensional filament studies by Hall-McNair et al. [18] and Walker et al. [15], the latter incorporating a planar no-slip boundary and still yielding an explicit linear relation analogous to Eq. (18).

Combining Eqs. (13), (18) and (19) yields the linear system
\begin{align}
-\mathcal{B} \begin{bmatrix} A^{-1} & 0 \\ 0 & \hat{A} \end{bmatrix} \begin{bmatrix} \dot{X} \\ \dot{\omega} \end{bmatrix} = -\mathcal{B} A \begin{bmatrix} \dot{X} \\ \dot{\omega} \end{bmatrix} = R, \tag{20}
\end{align}
where we are assuming that $A$ is invertible and defining $\hat{A}$ to be a block matrix of dimension $(6N + 3) \times (4N + 3)$ with non-zero blocks $A^{-1}$ and $\hat{A}$.

**Parameterisation**

We may parameterise the tangents $d_3^i$ on each linear segment by the Euler angles $\theta_i \in [0, \pi]$ and $\phi_i \in (-\pi, \pi]$.
for \( i = 1, \ldots, N \) [21]. With this parameterisation we may make a choice of \( d_1 \) and \( d_2 \), taking here the three orthonormal vectors to be

\[
d_1 = [-s_\phi c_\psi - c_\phi c_\psi s_\psi, +c_\phi c_\psi - c_\phi s_\psi s_\psi, s_\phi s_\psi]^T, \tag{21}
\]
\[
d_2 = [+s_\phi c_\psi - c_\phi c_\psi s_\psi, -c_\phi c_\psi - c_\phi s_\psi s_\psi, s_\phi s_\psi]^T, \tag{22}
\]
\[
d_3 = [s_\phi c_\psi, s_\phi s_\psi, c_\phi]^T, \tag{23}
\]

written with respect to the laboratory frame and where \( s_\theta \equiv \sin \theta_1 \), \( c_\theta \equiv \cos \theta_1 \), and analogously for \( s_\phi \), \( c_\phi \), \( s_\psi \) and \( c_\psi \). From the directors we recover

\[
\theta_i = \arccos \left( d_3^i \cdot e_z \right), \tag{24}
\]
\[
\phi_i = \arctan \left( \frac{d_2^i \cdot e_y}{d_3^i \cdot e_x} \right), \tag{25}
\]
\[
\psi_i = \arctan \left( \frac{d_1^i \cdot e_z}{d_2^i \cdot e_z} \right). \tag{26}
\]

As the discretised filament is piecewise linear, for \( j = 1, \ldots, N + 1 \) we may write

\[
x_j = x_1 + \Delta s \sum_{i=1}^{j-1} d_3^i, \tag{27}
\]
\[
\dot{x}_j = \dot{x}_1 + \Delta s \sum_{i=1}^{j-1} d_3^i. \tag{28}
\]

With \( d_3^i \) parameterised as above, we can thus express \( \dot{x}_j \) as a linear combination of the derivatives of \( \theta_i \) and \( \phi_i \) for \( i = 1, \ldots, j - 1 \), in addition to including the time derivative of the base point \( x_1 \). Hence we may write

\[
\dot{\Theta} = \dot{X}, \tag{29}
\]
\[
\Theta = [x_{1,x}, x_{1,y}, x_{1,z}, \theta_1, \ldots, \theta_i, \ldots, \psi_1, \ldots, \psi_N]^T, \tag{30}
\]

where \( Q \) is a 3(\( N + 1 \)) \times 3(\( N + 1 \)) matrix and \( x_{1,x}, x_{1,y}, x_{1,z} \) are the components of \( x_j \) in the basis \( \{ e_x, e_y, e_z \} \). Explicitly, \( Q \) may be constructed as

\[
Q = \begin{bmatrix}
Q_{11} & Q_{12} & Q_{13} \\
Q_{21} & Q_{22} & Q_{23} \\
Q_{31} & Q_{32} & Q_{33}
\end{bmatrix}, \tag{31}
\]

where the matrices \( Q_{kl} \) are of dimension \((N + 1) \times 3\), with \( Q_{k2} \) and \( Q_{k3} \) being of dimension \((N + 1) \times N\), for \( k = 1, 2, 3 \). The subscript \( P \) denotes that the \( i \)th row of \( Q \) is to be permuted to

\[
P(i) = \begin{cases}
3(i - 1) + 1, & i = 1, \ldots, N + 1, \\
3(i - N - 2) + 2, & i = N + 2, \ldots, 2N + 2, \\
3(i - 2N - 3) + 3, & i = 2N + 3, \ldots, 3N + 3.
\end{cases} \tag{32}
\]

This permutation of \( Q \) allows us to define the sub-blocks of \( Q \) simply, given explicitly as

\[
Q_{ki} = \begin{cases}
1, & j = k, \\
0, & \text{otherwise},
\end{cases} \tag{33}
\]

where

\[
Q_{12} = \begin{cases}
+ \cos \theta_j \cos \phi_j, & j < i, \\
0, & j \geq i,
\end{cases} \tag{34}
\]

\[
Q_{13} = \begin{cases}
- \sin \theta_j \sin \phi_j, & j < i, \\
0, & j \geq i,
\end{cases} \tag{35}
\]

Further, in this parameterisation we may relate the local rate of rotation \( \omega \) about \( d_3^i \) to \( \theta, \phi, \psi \) and their time derivatives. Explicitly, this relationship is given by

\[
Q = \begin{bmatrix}
\dot{X} \\
0
\end{bmatrix}, \tag{36}
\]

where \( I_N \) is the \( N \times N \) identity matrix and the \( N \times N \) matrix \( C \) has diagonal elements \( C_i = \cos(\theta_i) \) for \( i = 1, \ldots, N \), with all other elements zero. The \((4N + 3) \times 3(N + 1)\) matrix \( Q \) now encodes the expressions of velocities and rotation rates in terms of the parameterisation, via

\[
- \dot{R}A Q \dot{\Theta} = \dot{R}, \tag{37}
\]

noting in particular that the matrix \( A \) is square and has dimension \((3N + 3) \times (3N + 3)\). Naively, this system of ordinary differential equations can be readily solved numerically to give the evolution of the filament in the surrounding fluid. However, the use of a single parameterisation to describe the filament will in general lead to degeneracy of the linear system and ill-defined derivatives in both space and time, issues which we explore and resolve numerically in the next section.

**Coordinate singularities**

Consider a straight filament aligned with the \( e_z \) axis, with each of the \( d_3^i = [0, 0, 1]^T \) written in the
laboratory frame. For this filament $\theta_i = 0$ for all $i$, whilst the $\phi_i$ are undetermined, arbitrary and notably need not be the same on each segment. Were we to attempt to formulate and solve the linear system of Eq. (35), both $\phi$ and its derivatives would be ill-defined, and correspondingly we would be unable to solve the system for the filament dynamics, which are otherwise trivial in this particular setup. In more generality, if a filament were to have any segment pass through one of the poles $\theta = \{0, \pi\}$ of this coordinate system, $\phi$ would be undetermined on the segment and arbitrary, with attempts to solve our parameterised system of ordinary differential equations failing. Further, were a segment to pass close to but not through a pole, with attempts to solve our parameterised system of ordinary differential equations would be undetermined on the segment and arbitrary, the value of $\phi$ varying rapidly and artificially between varying rapidly and artificially between.

An analogous issue with arclength derivatives occur when considering neighbouring segments, with the value of $\phi$ varying rapidly and artificially between segments that reside near the pole of the coordinate system. In this latter case however, our formulation of the elastohydrodynamical problem circumvents the need for evaluation of $\phi_s$, instead considering only derivatives of the smooth quantities $d_s$, though we are not able to resolve issues with temporal derivatives in the same way.

In order to avoid the numerical and theoretical problems associated with singular points in the filament parameterisation, we exploit the finiteness of the set of angles $\theta_i$ along with the independence of the underlying elastohydrodynamical problem from the parameterisation. Throughout this work we have assumed a fixed laboratory frame with basis $\{e_x, e_y, e_z\}$, present only so that vector quantities may be written componentwise for convenience. Our choice of such a basis is arbitrary, with the physical problem of filament motion being independent of our selection of particular basis vectors. It is with respect to this basis that we have defined the Euler angles $\theta$ and $\phi$, from which the aforementioned coordinate singularities appear if any of the $\theta_i$ approach zero or $\pi$. Thus, if one makes a choice of basis $\{e^*_x, e^*_y, e^*_z\}$ such that the corresponding Euler angles $\theta^*_i$ are some $\delta$-neighbourhood away from the poles of the new parameterisation, the system of ordinary differential equations given in Eq. (35) may be readily solved, at least initially. Should the solution in the new coordinate system approach one of the new poles $\theta^* = 0, \pi$, a new basis can again be chosen, and this process iterated until the filament motion has been captured over a desired interval.

We note that for sufficiently large $\delta > 0$ such a choice of basis $\{e^*_x, e^*_y, e^*_z\}$ necessarily exists due to the finiteness of the set of $\theta_i$, with $\delta$ in practice able to be sufficiently large so as to limit the effects of coordinate singularities. Thus, subject to reasonable assumptions of smoothness of the filament position $x$, such a process of repeatedly changing basis when necessary will prevent issues associated with the parameterisation described above, and will in practice enable the efficient simulation of filament motion without introducing artificial stiffness or singularities.

**IMPLEMENTATION AND VERIFICATION**

Initially choosing a random basis $\{e_x, e_y, e_z\}$, the above formulation is implemented in MATLAB, with the system of ordinary differential equations of Eq. (35) being solved using the inbuilt stiff ODE solver ode15s [22], making use of variable step sizes in order to satisfy configurable error tolerances that are typically set here at $10^{-7}$. Initially and at each timestep, the values of $\theta_i$ are checked to determine if they are within $\delta$ of a coordinate singularity, typically with $\delta = \pi / 30$. Should the parameterisation be approaching a singularity, a new basis is chosen and the problem recast in this basis.

A natural method of selecting a new basis is to choose one uniformly at random. Indeed, by considering the worst-case scenario of the $N$ tuples $(\theta_i, \phi_i)$ uniformly and disjointly covering the surface of the unit sphere, which together $\theta$ and $\phi$ parameterise, the probability that any random basis results in $\min_i |\theta_i - \pi - \pi | < \delta$ is given by $2N \sin^2(\delta / 2)$, a consequence of elementary geometry. With this quantity being significantly less than unity for a wide range of $N$ with $\delta$ large enough to avoid severe artificial numerical stiffness, as discussed above, a practical implementation for the simulation of filament elastohydrodynamics as formulated above may simply select a new basis randomly, repeating until a suitable basis is found. With $\delta = \pi / 50$ and $N = 50$, the probability of needing to select another basis is bounded above by $10\%$, thus in practice one should expect to find an appropriate basis within few iterations of the proposed procedure.

However, we may proceed in a deterministic manner, selecting an appropriate basis from knowledge of the existing parameterisation. Given the set of parameters $\theta_i$ and $\phi_i$, we may choose a $\theta \in [0, \pi]$ so as to maximise the distance of $\theta$ from the poles $\theta = 0, \pi$ of the existing system, as well as from each of the $\theta_i$ and their antipodes, $\pi - \theta_i$. Similarly, we may choose $\phi \in (-\pi, \pi)$ so as to maximise the distance from each of the $\phi_i$ and their antipodes, where distance is measured modulo $2\pi$. With these choices of $\theta$ and $\phi$, we form a new basis by mapping the original basis vector $e_x$ to the vector $e^*_x$, given explicitly by

$$e^*_x = [\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta]^\top.$$  

Choosing the other orthonormal basis vectors $e^*_y, e^*_z$
FIG. 1. The relaxation of a filament in three dimensions. Shown are the initial (left) and relaxed (right) configurations of the filament (black, heavy). The vectors $d_i^\alpha$ are shown as coloured arrows for particular values of $i$ and $\alpha = 1, 2$. We see relaxation from a non-planar, highly-twisted configuration to a straight filament, with intermediate transients during which the filament untwists and unbends not shown. Here we have simulated filament motion with $N = 100$ segments and $\sigma = 1$.

arbitrarily, expressed in this new basis the accompanying filament parameterisation will be removed from any coordinate singularities, by construction. By considering the $\phi_i$ and not simply the $\theta_i$ alone, we have further increased the separation between the filament parameterisation and coordinate singularities.

Utilising the above deterministic scheme for basis selection, typical simulations of filament relaxation in three dimensions utilising $N = 80$ segments have an average runtime of approximately 60s on modest hardware (Intel® Core™ i7-6920HQ CPU), typically requiring at most one random choice of basis to avoid singularities in the parameterisation, though this latter observation is naturally configuration-dependent. We see retained in this methodology the low computational cost of the formulation of Moreau et al. [14], here extended to filaments in three dimensions and representing significant improvements in computational efficiency over recent studies in three dimensions [12, 13].

Initial verification was performed by comparison to filament relaxation in two dimensions [14, 16], along with repeated observation of the relaxation of a variety of initially-curved filaments relaxing in three dimensions to a straight configuration. An example of such a filament and its relaxation to a straight configuration is given in Fig. 1 notably beginning from a highly-twisted configuration passing close to the poles of the laboratory-based Euler angle parameterisation of the filament as shown in the figure.

DISCUSSION

We have seen that the motion of inextensible unshearable filaments in three dimensions can be concisely described by an Euler angle parameterisation suitable for efficient numerical solution. Further, we have found that singularities introduced by a choice of coordinate system may be readily circumvented by a change of basis, avoiding artificial numerical stiffness and potential degeneracies in any single parameterisation of the filament. We have extended the two-dimensional methodologies of Moreau et al. [14], Walker et al. [15], Hall-McNair et al. [16] to consider non-planar filaments, and have retained the computational efficiency associated with these previous studies, potentially enabling large-scale exploratory studies of filament dynamics that were previously plagued by severe numerical stiffness.

Though not detailed in this manuscript, the presented framework may readily accommodate hydrodynamics in confined geometries, for example with the inclusion of a planar boundary as in Walker et al. [15], in addition to non-trivial background flows, active moments, and complex boundary conditions. Such a framework will enable the study of filament dynamics relevant to biological applications as well as to active matter, a pertinent example being the flagellum of the mammalian spermatozoon.

ACKNOWLEDGEMENTS

We are grateful to Prof. Derek Moulton for discussions on elastic filaments, and to Prof. David Smith for discussions on basis rotation. B.J.W. is supported by the UK Engineering and Physical Sciences Research Council (EPSRC), grant EP/N509711/1. K.I. is supported by JSPS Overseas Research Fellowship (29-0146), MEXT Leading Initiative for Excellent Young Researchers (LEADER), and JSPS KAKENHI Grant Number JP18K13456.

* Corresponding author: benjamin.walker@maths.ox.ac.uk
† ishimoto@ms.u-tokyo.ac.jp
‡ gaffney@maths.ox.ac.uk

[1] H. C. Berg and R. A. Anderson, Bacteria Swim by Rotating their Flagellar Filaments, Nature 245, 380 (1973).
[2] J. Gray, Ciliary movement (Cambridge University Press, Cambridge [England, 1928).
[3] D. J. Smith, T. D. Montenegro-Johnson, and S. S. Lopes, Symmetry-Breaking Cilia-Driven Flow in Embryogenesis, Annual Review of Fluid Mechanics 51, 105 (2019).
[4] L. Guglielmini, A. Kushwaha, E. S. G. Shaqfeh, and H. A. Stone, Buckling transitions of an
elastic filament in a viscous stagnation point flow, 
Physics of Fluids 24, 123601 (2012)

[5] M. Roper, R. Dreyfus, J. Baudry, M. Fermigier, J. Bibette, and H. A. Stone, On the dynamics of magnetically driven elastic filaments, 
Journal of Fluid Mechanics 554, 167 (2006)

[6] A. K. Tornberg and M. J. Shelley, Simulating the dynamics and interactions of flexible fibers in Stokes flows, 
Journal of Computational Physics 196, 8 (2004)

[7] Y. Liu, B. Chakrabarti, D. Saintillan, A. Lindner, and O. du Roure, Morphological transitions of elastic filaments in shear flow, 
Proceedings of the National Academy of Sciences 115, 9438 (2018)

[8] C. Pozrikidis, Shear flow over cylindrical rods attached to a substrate, 
Journal of Fluids and Structures 26, 393 (2010)

[9] O. du Roure, A. Lindner, E. N. Nazockdast, and M. J. Shelley, Dynamics of Flexible Fibers in Viscous Flows and Fluids, 
Annual Review of Fluid Mechanics 51, 539 (2019)

[10] S. F. Schoeller, A. K. Townsend, T. A. Westwood, and E. E. Keaveny, Methods for suspensions of passive and active filaments, 
, 1 (2019) arXiv:1903.12809

[11] M. Maxey and B. Patel, Localized force representations for particles sedimenting in Stokes flow, 
International Journal of Multiphase Flow 27, 1603 (2001)

[12] S. D. Olson, S. Lim, and R. Cortez, Modeling the dynamics of an elastic rod with intrinsic curvature and twist using a regularized Stokes formulation, 
Journal of Computational Physics 238, 169 (2013)

[13] K. Ishimoto and E. A. Gaffney, An elastohydrodynamical simulation study of filament and spermatozoan swimming driven by internal couples, 
IMA Journal of Applied Mathematics 83, 655 (2018)

[14] C. Moreau, L. Giraldi, and H. Gadelha, The asymptotic coarse-graining formulation of slender-rods, bio-filaments and flagella, 
Journal of The Royal Society Interface 15, 20180235 (2018)

[15] B. J. Walker, K. Ishimoto, H. Gadelha, and E. A. Gaffney, Filament mechanics in a half-space via regularised Stokeslet segments, 
(2019) arXiv:1904.02543

[16] A. L. Hall-McNair, M. T. Gallagher, T. D. Montenegro-Johnson, H. Gadelha, and D. J. Smith, Efficient Implementation of Elastohydrodynamics via Integral Operators, 
, 1 (2019) arXiv:1903.03427

[17] M. Nizette and A. Goriely, Towards a classification of Euler-Kirchhoff filaments, 
Journal of Mathematical Physics 40, 2830 (1999)

[18] G. J. Hancock, The self-propulsion of microscopic organisms through liquids, 
Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences 32, 802 (1955)

[19] A. Chwang and T. Y.-T. Wu, Hydromechanics of low-Reynolds-number flow. Part 1. Rotation of axisymmetric prolate bodies, 
Journal of Fluid Mechanics 63, 607 (1974)

[20] S. S. Antman, [Nonlinear Problems of Elasticity], Applied Mathematical Sciences, Vol. 107 (Springer-Verlag, New York, 2005).

[21] J. Gray and G. J. Hancock, The Propulsion of Sea-Urchin Spermatozoa, Journal of Experimental Biology 32, 802 (1955)

[22] L. F. Shampine and M. W. Reichelt, The MATLAB ODE Suite, 
SIAM Journal on Scientific Computing 18, 1 (1997)