A fully three-dimensional model of the interaction of driven elastic filaments in a Stokes flow with applications to sperm motility

Julie Simons^a, Lisa Fauci^a, Ricardo Cortez^a

^a*Center for Computational Science and Mathematics Department, Tulane University,
6823 St. Charles Ave., New Orleans, LA 70118, USA*

Abstract

In many animals, sperm flagella exhibit primarily planar waveforms. An isolated sperm with a planar flagellar beat in a three-dimensional unbounded fluid domain would remain in a plane. However, because sperm must navigate through complex, three-dimensional confined spaces along with other sperm, forces that bend or move the flagellum out of its current beat plane develop. Here we present an extension of previous models of an elastic sperm flagellar filament whose shape change is driven by the pursuit of a preferred curvature wave. In particular, we extend the energy of the generalized elastica to include a term that penalizes out-of-plane motion. We are now able to study the interaction of free-swimmers in a 3D Stokes flow that do not start out beating in the same plane. We demonstrate the three-dimensional nature of swimming behavior as neighboring sperm swim close to each other and affect each others' trajectories via fluid-structure coupling.

Keywords: Sperm motility, three-dimensional flagellum, planar waveforms,

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Email addresses: `jsimons@tulane.edu` (Julie Simons), `fauci@tulane.edu` (Lisa Fauci), `rcortez@tulane.edu` (Ricardo Cortez)

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1. Introduction

For successful fertilization, sperm must be able to navigate complex environments to reach the egg. Thus, sperm motility patterns are vital components of sexual reproduction. In many species, sperm flagellar waveforms are planar or near-planar, though helical waveforms are also stable [48, 51]. Planar waveforms of an isolated beating flagellum result in trajectories that are characterized by either linear or circular paths within the plane, depending on the symmetry of the beat pattern [36, 52]. However, forces exerted on the planar swimmer by proximal surfaces or nearby swimmers can easily bend or pull part or all of the flagellum out of its current beat plane.

Three-dimensional behavior of sperm flagella has been experimentally observed [50] and some species exhibit “figure 8” or helical deviations of the waveform out of the plane [10, 51]. More recent experimental advances in tracking sperm at a high resolution have exposed the three-dimensional nature of swimming trajectories of sperm in populations, providing experimental evidence for helical or “chiral ribbon” trajectories [7, 42, 43]. The recent review of Guerrero et al. [21] highlights the importance of understanding sperm motility in fully three-dimensional settings in order to correctly characterize and assess fertility in sperm.

The hydrodynamics of sperm motility is characterized by low Reynolds number, viscous fluid mechanics, and has been the inspiration of many classic studies in biological fluid dynamics [15], including G.I. Taylor’s swimming sheet [46] and the resistive force theory of Gray and Hancock [20]. In these

24 early models, the kinematics of the flagellar waveform were imposed, and the
 25 resulting swimming speed of the flagellum was calculated. Recognizing that
 26 a sperm flagellum is an elastic structure whose realized kinematics are de-
 27 termined by its coupling to the surrounding viscous fluid, models have been
 28 developed that treat the flagellum as a generalized Euler elastica, whose
 29 shape change is driven by the pursuit of a preferred curvature wave [17].
 30 Such flagellar models, essentially of swimming sheets, have been coupled to
 31 a two-dimensional fluid and have been used to study synchronization of finite
 32 swimmers and their attraction to walls [16], and the effect of viscoelasticity
 33 on flagellar swimming [6, 47]. More recently, these driven-elastica have been
 34 coupled to a model for three-dimensional Stokes flow and have been used to
 35 study the emergence of a hyperactivated waveform due to calcium dynamics
 36 in a single, isolated flagellar filament [34], and the elastic attachment of a
 37 planar flagellar filament to an orthogonal planar wall [40]. While the dynam-
 38 ics of these filaments were coupled to a three-dimensional domain of fluid,
 39 the symmetry imposed by a single flagellum confined to a plane in free-space
 40 or one beating perpendicular to an infinite planar wall does not result in any
 41 out-of-plane component of force on the flagellum.

42 Motivated by the understanding sperm-sperm and sperm-boundary in-
 43 teractions in more general settings, even for driven filaments that pursue a
 44 planar waveform, here we extend the generalized Euler elastica energy formu-
 45 lation of [17] to include a penalty for out-of-plane motion. The native flagellar
 46 plane will evolve in time. The energy that drives this new model is rotation-
 47 and translation-invariant, therefore the filament will be a free-swimmer that
 48 generates zero total force and torque.

While several different mathematical approaches may be used to couple flagellar forces to a fluid, here we use the 3D method of regularized Stokeslets [9]. In the following sections, we present the mathematical formulation of the three-dimensional model, how to incorporate multiple nearby sperm, and then discuss the implications for three-dimensional trajectories and behaviors in sperm populations.

2. Methods

2.1. Derivation of the Three-Dimensional Model

We model the sperm flagellum as a three-dimensional curve $\mathbf{X}(s, t)$ that exerts forces along its length in a viscous fluid governed by the incompressible Stokes equations:

$$\begin{aligned}\mu\Delta\mathbf{u} &= \nabla p - \int_0^L \mathbf{f}(\mathbf{X}(s, t), t)\phi_\epsilon(\mathbf{x} - \mathbf{X}(s, t))ds \\ \nabla \cdot \mathbf{u} &= 0\end{aligned}\tag{1}$$

where L is the total length of the flagellum, s is arc length, t is time, μ is the dynamic viscosity, $\mathbf{u}$ is fluid velocity, and p is the pressure. The forces $\mathbf{f}(\mathbf{X}, t)$ exerted by the flagellum upon the surrounding fluid are regularized by a blob function ϕ_ϵ defined by:

$$\phi_\epsilon(r) = \frac{15\epsilon^4}{8\pi(r^2 + \epsilon^2)^{7/2}}.$$

This is a regularized delta function that distributes the force in a small fluid volume around the curve [8, 9]. This regularization eliminates singularities in the velocity field and the parameter ϵ is chosen to be on the order of the diameter of the sperm flagellum. The flagellum will be considered an

68 immersed boundary that moves with the fluid velocity at all points along its
69 length.

70 Our model assumes that sperm flagella have a nearly planar beat. Both
71 helical and planar flagellar beat forms may be stable. Planar waveforms may
72 be more prevalent near surfaces and observed helical waveforms may in fact
73 be more aptly described as “flattened helices” [4, 37, 51]. The planar or
74 quasi-planar nature of the sperm flagellum is most likely controlled by the
75 structure of the microtubule doublets and dynein bridges of the axoneme [19,
76 22, 26, 27, 35, 39]. We do not seek to model the underlying structure of the
77 flagellum nor how a planar preference might arise, but instead conceptualize
78 the sperm flagellum as a thin filament that would naturally have a planar
79 shape in the absence of external forces.

80 This extended model is formulated so that a flagellum can accommodate
81 three-dimensional effects that cause deviations from planar configurations.
82 These effects could include surfaces, other sperm swimming nearby, or other
83 external forces. To accomplish this, we incorporate forces that restrict out-
84 of-plane deviations of the flagellum. Within the flagellar plane, we prescribe
85 curvature-based forces along the flagellum as in [17], which enable the sperm
86 to move in a wave-like manner.

87 The forces $\mathbf{f}$ will be derived using a continuous energy formulation that
88 is an extension of the internally-actuated filament model in [17]. In order
89 to define the energy, we first define a local coordinate system in which the
90 flagellar plane is $z = 0$. This will be referred to as the flagellum frame
91 of reference. In this frame of reference, bending forces that modulate the
92 swimming behavior of the flagellum will occur in the plane $z = 0$ alone.

Moreover, non-planar deviations can be understood as deviations in the z component and forces restricting these deviations can be found. For clarity, in the flagellum frame of reference, we refer to the Cartesian coordinates as $\hat{x}, \hat{y}$, and $\hat{z}$ and the coordinates of the flagellum itself as $\hat{\mathbf{X}}$. Thus the flagellar plane is the plane $\hat{z} = 0$.

Using this notation, we define the total energy as:

$$\mathcal{E}(\hat{\mathbf{X}}, t) = \mathcal{E}_{tens}(\hat{\mathbf{X}}, t) + \mathcal{E}_{bend}(\hat{\mathbf{X}}, t) + \mathcal{E}_{plane}(\hat{\mathbf{X}}, t)$$

where $\mathcal{E}_{tens}$ is a tensile energy term that enforces inextensibility, $\mathcal{E}_{bend}$ is a time-dependent bending energy that drives the beating behavior of the filament, and $\mathcal{E}_{plane}$ is the energy arising from out-of-plane deviations. Each energy is defined as follows:

$$\mathcal{E}_{tens}(\hat{\mathbf{X}}, t) = \frac{1}{2} S_t \int_0^L \left[\left\| \frac{\partial \hat{\mathbf{X}}}{\partial s} \right\| - 1 \right]^2 ds \quad (2)$$

$$\mathcal{E}_{bend}(\hat{\mathbf{X}}, t) = \frac{1}{2} S_b \int_0^\ell \left[\left(\frac{\partial \hat{\mathbf{X}}}{\partial \alpha} \times \frac{\partial^2 \hat{\mathbf{X}}}{\partial \alpha^2} \right) \cdot \mathbf{e}_3 - C(\alpha, t) \right]^2 d\alpha \quad (3)$$

$$\mathcal{E}_{plane}(\hat{\mathbf{X}}, t) = \frac{1}{2} S_p \int_0^L \left[\frac{\partial \hat{\mathbf{X}}}{\partial s} \cdot \mathbf{e}_3 \right]^2 ds \quad (4)$$

where S_i are stiffness coefficients, L is the length of the flagellum, and $\mathbf{e}_3 = (0, 0, 1)^T$ is the normal to the flagellar plane. The function $C(\alpha, t)$ is the preferred curvature that drives the swimming motion of the sperm. Since this function is restricted to the plane $\hat{z} = 0$, the parameter α refers to the projection of the filament arc length onto that plane, and ℓ is the total projected arc length in that plane. We take ℓ to be approximately constant because deviations from the plane are assumed to be small.

106 With these definitions, the energies (2) and (3) are the same energies
 107 described in [17] and the energy (4) is the new addition to our model. The
 108 energy (4) is non-zero when there are local deviations of the flagellum in
 109 the $\hat{z}$ direction (i.e. deviations from the flagellar plane). The total energy
 110 $\mathcal{E}$ is translation- and rotation-invariant and forces in the flagellum frame of
 111 reference $\hat{\mathbf{f}}$ can be calculated as

$$\hat{\mathbf{f}} = -\frac{\partial \mathcal{E}}{\partial \hat{\mathbf{X}}}.$$

112 These resulting forces seek to minimize the total energy, where the tensile,
 113 bending and planarity stiffness constants (S_t, S_b, S_p) determine how closely
 114 the preferred planar traveling wave is realized. In particular, the tensile stiff-
 115 ness S_t is chosen large enough so that the filament is effectively inextensible,
 116 the bending stiffness S_b reflects the bend modulus of the flexible filament,
 117 and the planarity stiffness S_p controls the penalty for deviation from the
 118 plane. Finding the forces $\mathbf{f}$ in the original frame of reference requires a trans-
 119 formation from the $(\hat{x}, \hat{y}, \hat{z})$ coordinates to the global Cartesian coordinates
 120 (x, y, z) .

121 For computational purposes, we will discretize the integral in (1) by defin-
 122 ing discrete points $\mathbf{X}_k$ along the flagellum (where k denotes the index of the
 123 point). Figure 1 shows a schematic of the physical domain of the discretized
 124 flagellum for a preferred sinusoidal waveform with amplitude b .

125 Using the method of regularized Stokeslets described in [9], the fluid ve-
 126 locity is given by

$$\mathbf{u}(\mathbf{x}) = \sum_k \frac{r_k^2 + 2\epsilon^2}{(r_k^2 + \epsilon^2)^{3/2}} \mathbf{f}_k + \frac{(\mathbf{f}_k \cdot (\mathbf{x} - \mathbf{X}_k)) (\mathbf{x} - \mathbf{X}_k)}{(r_k^2 + \epsilon^2)^{3/2}}$$

127 where $r_k = \|\mathbf{x} - \mathbf{X}_k\|$ and ϵ is set to be close to the flagellum diameter. The
 128 points will be discretized so that their spacing is less than ϵ . The discrete
 129 forces $\mathbf{f}_k$ define the forces the flagellum exerts at points $\mathbf{X}_k$, and are calculated
 130 from discretized versions of the energies (2)-(4). The motion of the flagellum
 131 points is described by the equation

$$\frac{d\mathbf{X}_k}{dt} = \mathbf{u}(\mathbf{X}_k(t), t)$$

132 which is approximated using a forward Euler method. In the next several sec-
 133 tions, we describe the specific components of the three-dimensional preferred
 134 curvature model.

135 2.2. Derivation of the discrete flagellar plane bending energy

136 We discretize the bending energy (3), as in [17]:

$$E_{bend,xy} = \frac{1}{2}S_b \sum_{k=2}^{N-1} \left(\frac{(\hat{x}_{k+1} - \hat{x}_k)(\hat{y}_k - \hat{y}_{k-1}) - (\hat{y}_{k+1} - \hat{y}_k)(\hat{x}_k - \hat{x}_{k-1})}{\Delta\alpha^3} - C_k(t) \right)^2 \Delta\alpha \quad (5)$$

137 where S_b is the bending stiffness constant, N is the total number of points
 138 along the flagellum, and $\Delta\alpha$ is a constant equal to the desired spacing
 139 between the points $(\hat{x}_k, \hat{y}_k, 0)$. The preferred curvature $C_k(t)$ is a time-
 140 dependent sinusoidal function similar to the one used in [17]:

$$C_k(t) = \kappa^2 b \sin(\kappa\alpha_k - \omega t) \quad (6)$$

141 where α_k is the arc length distance along the flagellum (projected onto the
 142 plane $\hat{z} = 0$) from the head point $(\hat{x}_1, \hat{y}_1, 0)$ up to the point $(\hat{x}_k, \hat{y}_k, 0)$, and
 143 κ and ω are the wavenumber and frequency parameters, respectively. In
 144 this model, we choose $\kappa = \frac{2\pi}{L}$ so there is approximately one wavelength per
 145 flagellum length, but our results are not qualitatively sensitive to this choice.

Small out-of-plane deviations of the flagellum imply that $\Delta\alpha$ may be smaller but not too different from Δs (the desired spacing between points in 3D). In order not to overestimate the desired planar curvature forces for three-dimensional flagellar configurations, we consider the three-dimensional vector of length Δs given by

$$\mathbf{r}_{k+1} = \Delta s \frac{\hat{\mathbf{X}}_{k+1} - \hat{\mathbf{X}}_k}{\|\hat{\mathbf{X}}_{k+1} - \hat{\mathbf{X}}_k\|},$$

and define $\Delta\alpha_{k+1}$ as the length of the projection of vector $\mathbf{r}_{k+1}$ onto the flagellar plane:

$$\Delta\alpha_{k+1} := \|\mathbf{r}_{k+1} - (\mathbf{e}_3 \cdot \mathbf{r}_{k+1})\mathbf{e}_3\|.$$

With this definition, the factors of $\Delta\alpha^3$ and $\Delta\alpha$ in Eq. (5) are replaced with

$$\Delta\alpha^3 \rightarrow \Delta\alpha_k \Delta\alpha_{k+1} \frac{\Delta\alpha_k + \Delta\alpha_{k+1}}{2}, \quad \Delta\alpha \rightarrow \frac{\Delta\alpha_k + \Delta\alpha_{k+1}}{2} \quad (7)$$

We note that $\Delta\alpha_k = \Delta s$ for all k when the points are exactly in the plane $\hat{z} = 0$.

2.3. Plane restriction force

To address out-of-plane deviations, we discretize the energy (4) as:

$$E_{plane} = \frac{1}{2} S_p \sum_{k=1}^{N-1} \left(\frac{\hat{z}_{k+1} - \hat{z}_k}{\Delta s} \right)^2 \Delta s.$$

This energy formulation restricts any non-planar deviations via forces in the $\hat{z}$ -direction but is a local effect that seeks to minimize the total quadratic variation in $\hat{z}$, hence reducing the concavity of $\hat{z}(s)$. The force derived from this energy acting upon an interior point $k \in (2, \dots, N-1)$ would then be:

$$\hat{\mathbf{f}}_k = S_p (\hat{z}_{k+1} - 2\hat{z}_k + \hat{z}_{k-1}) \frac{1}{\Delta s} \mathbf{e}_3 \approx S_p \Delta s \hat{z}''(s_k) \mathbf{e}_3. \quad (8)$$

162 Because the energy function E_{plane} , like the bending and tensile energies, is
 163 rotationally- and translationally-invariant, the net force and the net torque
 164 due to E_{plane} satisfy:

$$\sum_k \hat{\mathbf{f}}_k = \sum_k \hat{\mathbf{X}}_k \times \hat{\mathbf{f}}_k = \mathbf{0}.$$

165 This can be proven by direct calculation from (8) and is due to Noether's
 166 Theorem [1]. These two conditions on the net force and net torque are
 167 constraints required for self-propelled organisms.

168 2.4. *Incorporating asymmetry*

Motility patterns in sperm are typically characterized as active (symmet-
 ric) or hyperactive (asymmetric with high amplitude). Because hyperactivity
 is required for successful fertilization of the egg [44, 45, 52], we consider both
 asymmetric and symmetric preferred beat-forms. To incorporate asymmetry
 into this model, we use a simple amplitude modulation approach as in [34] to
 set the preferred curvature function $C_k(t)$ in expression (6) along the flagel-
 lum for all times t . For our flagellum of length $100 \mu\text{m}$, we let the amplitude
 b of the curvature function (6) take the following values:

$$b = \begin{cases} b_1 & \text{if } \sin(\kappa s_k - \omega t) < 0 \\ b_2 & \text{if } \sin(\kappa s_k - \omega t) \geq 0. \end{cases} \quad (9)$$

169 In the case of a symmetric waveform, we choose $b_1 = b_2 = 10 \mu\text{m}$. To explore
 170 the effect of a weak asymmetry in curvature, we choose $b_1 = 10 \mu\text{m}$ and $b_2 =$
 171 $15 \mu\text{m}$. For a stronger, higher amplitude asymmetry we choose $b_1 = 10 \mu\text{m}$
 172 and $b_2 = 25 \mu\text{m}$. The stronger asymmetry parameters have been chosen such
 173 that the behavior is closer to the deeper bends characteristic of hyperactive
 174 sperm motility patterns (see previous models in [34, 40]).

175 2.5. Defining the Flagellum Frame of Reference

176 At each time step, we need to update the preferred flagellar plane and
 177 flagellar frame of reference. We use the method of least squares, as described
 178 in [12], to define this plane. Given discrete points along the flagellum $\mathbf{X}_k$, we
 179 find the center of mass of the flagellum, denoted by $\bar{\mathbf{X}}$. This is simply the
 180 average position of all points $\mathbf{X}_k$. We define the flagellar plane as the plane
 181 that minimizes the sum of the squares of the orthogonal distances between
 182 the *centered* points $\mathbf{X}_k - \bar{\mathbf{X}} := (x_k, y_k, z_k)^T$ and the plane. The plane is
 183 represented by the vector $\mathbf{v} = (a, b, c)^T$, corresponding to least squares fit
 184 plane $ax + by + cz = 0$. We note that because the points (x_k, y_k, z_k) have
 185 zero average, this plane must go through the origin by construction.

186 The vector $\mathbf{v}$ defines the normal to the flagellar plane. This is equivalent
 187 to the $\hat{z}$ coordinate direction in the local (Lagrangian) flagellum frame of
 188 reference. Noting that a plane splits the space into two half-spaces, care
 189 is taken to ensure that $\mathbf{v}$ is always pointing towards the same half-space.
 190 This is important because the preferred curvature model in [17] requires the
 191 ability to discern the sign of the curvature. In other words, we must be
 192 able to choose between a plane normal vector pointing in the positive or
 193 negative $\hat{z}$ direction. Since our model is designed to represent a continuous
 194 process and we use a small numerical time step, the flagellar plane should
 195 not change significantly between time steps. Therefore, we add a check point
 196 in our algorithm that verifies that the normal vector from the previous time
 197 step and the normal vector from the current time step have a positive dot
 198 product.

199 Because forces within the flagellar plane are invariant under rotation and

translation, we may choose any $\hat{x}$ and $\hat{y}$ directions that would result in an orthonormal triad with $\mathbf{v}$ with the appropriate “right-hand rule” relationship between the coordinate directions. Figure 2 shows an example of a three-dimensional flagellum configuration, the least squares plane fit to the centered data, as well as the flagellum frame of reference.

2.6. Computational Method

In all simulations, each flagellum is initialized with a non-collinear configuration at time step $j = 0$ to ensure that a unique flagellar plane can be defined. The method for computing flagellar positions, forces, and velocities over time is as follows:

1. Calculate center of mass of flagellum points $\mathbf{X}_k$ and translate data so they have a center of mass at the origin.
2. Using the method of least squares, find the flagellar plane for centered flagellar data. The normal to this plane is represented by the normal vector $\mathbf{v}_j$.
3. For time step $j > 0$: if $\mathbf{v}_j \cdot \mathbf{v}_{j-1} < 0$, let $\mathbf{v}_j = -\mathbf{v}_j$ (signed curvature checkpoint).
4. Define $\hat{\mathbf{X}}_k$ using the flagellum frame of reference determined by $\mathbf{v}_j$.
5. Find forces $\hat{\mathbf{f}}_k$ for the points $\hat{\mathbf{X}}_k$ based on the total energy $\mathcal{E}$.
6. Rotate forces $\hat{\mathbf{f}}_k$ back to original frame of reference to obtain $\mathbf{f}_k$.
7. Solve for velocities $\mathbf{u}_k$ using the method of regularized Stokeslets and forces $\mathbf{f}_k$, as described in [34].
8. Move all points $\mathbf{X}_k$ using a forward Euler time step with velocities $\mathbf{u}_k$.
9. Let $j = j + 1$ and repeat.

224 2.7. Multiple Sperm

225 We are interested in how sperm trajectories are influenced by nearby
 226 neighbors. The model proposed here can consider any three-dimensional
 227 flagellum configuration with multiple sperm present. However, for realistic
 228 scenarios with multiple sperm, the model must not allow flagellum points to
 229 overlap. To address this, we add a repulsive force that acts on points that
 230 come within a certain distance of each other.

231 The repulsive force acting on the point $\mathbf{X}_k$ by the point $\mathbf{X}_j$ on separate
 232 flagellum will take the following form:

$$\mathbf{g}_k^j = S_r \left(\frac{1}{d} - \frac{1}{\min(r, d)} \right) (\mathbf{X}_k - \mathbf{X}_j) \quad (10)$$

233 where $r = \|\mathbf{X}_k - \mathbf{X}_j\|$ and d is a fixed distance. We choose this form because it
 234 is continuous in r and it tends to infinity as r approaches zero, which ensures
 235 that points do not get too close to one another if the time step is small.
 236 The choice of parameter S_r is arbitrary, but should be chosen so that the
 237 repulsion forces do not get too large too quickly (compared to the curvature
 238 forces) as r falls below d . The forces $\mathbf{g}_k^j$ will be added to the forces $\mathbf{f}_k$ before
 239 solving for velocities in the computational method. Note that contributions
 240 from this repulsion force maintain force- and torque-free swimming.

241 3. Results

242 Here we explore the effects of extending the elastica model of driven
 243 filaments to include an energy contribution for out-of-plane motion. In par-
 244 ticular, consider the cases of both a single planar flagellum swimming in 3D
 245 free-space, and a pair of coplanar flagella pursuing waves in that plane, whose

246 initial configurations are all planar. In these cases, the energy contribution
 247 for out-of-plane motion is always zero, and the trajectories of the swimmers
 248 remain in the initial plane. However, a pair of flagella each pursuing pla-
 249 nar waveforms in parallel planes will interact with each other and generate
 250 out-of-plane motion. Below we consider these cases, and also explore the
 251 consequences of out-of-plane perturbations of initial flagellar configurations
 252 in both an isolated flagellum and pairs of interacting flagella. All simula-
 253 tions use the model parameter values listed in Table 1 and were initialized
 254 with the flagellar configurations shown in Figure 3. The top row (Figure
 255 3a–3c) is used for coplanar or perturbed coplanar initial conditions, and the
 256 bottom row (Figure 3d–3f) is used for parallel plane initial configurations.
 257 From these small amplitude initial configurations (chosen for simplicity), the
 258 sperm flagellum evolves into its natural waveform over time. In all two sperm
 259 simulations presented here, the preferred curvature waves are specified to be
 260 in-phase. For further description of the method of regularized Stokeslets and
 261 scalings used for the fluid equations, please see [8, 40].

262 *3.1. Single Sperm*

263 We first consider a single flagellum that is pursuing a symmetric, planar
 264 wave, but whose initial small amplitude configuration is perturbed slightly
 265 out-of-plane. The flagellum was started with a primarily x - y sinusoidal planar
 266 conformation, with the head of the sperm slightly raised from the x - y plane
 267 (shown in black in Figure 3). We examine the dynamics of relaxation of this
 268 sperm flagellum to its native planar form from its initial three-dimensional
 269 configuration for various planarity stiffnesses S_p . The higher the value of
 270 this stiffness parameter, the faster one would expect the flagellum to relax

271 towards its native plane. The relaxation to the native flagellar plane can
 272 be characterized by considering the maximum value of $|\hat{z}_k|$ over all flagellum
 273 points. Figure 4 shows the relaxation behavior of this quantity over time
 274 for values of S_p between 0.001 and 1 pN μm^{-3} . We note that a value of 1
 275 is of the same order of magnitude as the inextensibility parameter connect-
 276 ing the flagellar points together. With this parameter value, the flagellum
 277 approaches its native plane within 10^{-4} s (or 10^{-3} beats). For symmetric
 278 waveforms, a single sperm would relax to a planar configuration and swim
 279 linearly forward within that plane. For an asymmetric waveform, the sperm
 280 would also relax to a planar configuration and swim in a circular motion
 281 within its native plane, as shown in Figure 9a and Movie M1.

282 3.2. *Two Sperm*

283 We examine the cases of two identical flagella pursuing in-phase planar
 284 waves in (a) the same plane and (b) parallel planes. The initial configurations
 285 are taken to be perfectly planar, with no perturbations (Figures 3a–3c with
 286 no perturbation from $z = 0$, and Figures 3d–3f). In the coplanar case, the
 287 sperm flagella attract and swim side by side, never leaving the plane $z = 0$.
 288 The trajectories for this scenario are shown in Figure 5a and Movie M2.
 289 Woolley et al. [49] demonstrated this attraction between bull spermatozoa in
 290 experiments where the swimming was confined to a glass surface. Numerical
 291 simulations using multi-particle collision dynamics in two dimensions by Yang
 292 et al. [53] and bead models in three dimensions by Llopis et al. [28] also
 293 demonstrate the attraction of nearby flagella.

294 In contrast, when two flagella are initialized in parallel planes, the flagella
 295 repel over time. This is shown by the trajectories in Figure 5b and the Movie

296 M3, where the two sperm are initially placed half a flagellum length ($50\ \mu\text{m}$)
 297 apart. Below, we will see that when they are placed closer together initially,
 298 the flagella may attract before ultimately repelling and swimming away from
 299 each other.

300 The velocities achieved by two identical interacting symmetric swimmers,
 301 when compared to an identically-actuated single swimmer, depend on relative
 302 distance and orientations of the flagella. The velocities versus minimum
 303 distance between the two flagella as a function of time are plotted in Figure
 304 6 for four different initial configurations of two swimmers that are pursuing
 305 identical symmetric waveforms, and whose planarity stiffness constant is $S_p =$
 306 1. Whereas a single swimmer has an average path velocity (i.e. the speed
 307 of the sperm over one beat period) of approximately $62\ \mu\text{m/s}$, the coplanar
 308 swimmers (Figure 5a) that are attracted towards each other have a decreased
 309 velocity of $50\ \mu\text{m/s}$ after they reach a steady swimming state (see Figure
 310 6c). The swimmers that start $50\ \mu\text{m}$ apart in parallel planes (see Figure
 311 5b) swim slower at all times, and approach a single swimmer's speed as
 312 they swim away from each other, as shown in Figure 6a. If the distance
 313 between initially parallel swimmers is reduced from $50\ \mu\text{m}$ to $5\ \mu\text{m}$, the
 314 swimmers actually see a transient increase in velocity and attract towards
 315 each other. They eventually do swim away from each other, however, even
 316 without a repelling force, as demonstrated in Figure 6b. The initial attraction
 317 of parallel swimmers, rotating their native plane and leading to an effective
 318 repulsion at longer times, is consistent with the observations of Llopis et al.
 319 [28].

320 Now we are going to consider perturbed coplanar initial configurations,

321 as depicted in Figures 3a–3c. Figure 7 through 9 and Movies M4–M7 show
 322 examples of two sperm swimming near each other with variations in the
 323 symmetry of the preferred curvature waveform. In particular, Figure 7 shows
 324 the relative motions of the sperm bodies for the two symmetric swimmers over
 325 a period of 10 seconds. Initially, the two sperm are swimming side-by-side in
 326 slightly different planes (labeled by $t = 0.1$ seconds). As time progresses, the
 327 sperm are attracted towards each other (labeled by $t = 5.1$ seconds) and then
 328 move away from each other (labeled by $t = 10.1$ seconds). The trajectories
 329 of the heads of these two swimmers are shown in Figure Figure 8a. While
 330 near each other, the fluid-structure coupling of the two sperm causes each
 331 filament to impact the trajectory (and preferred flagellar plane) of the other.
 332 The supplementary Movie M4 shows the swimming behavior of this pair of
 333 perturbed coplanar swimmers.

334 Although two perfectly coplanar swimmers pursuing a planar waveform
 335 would remain in that plane, this simulation shows that a small initial per-
 336 turbation from that plane is never recovered. As is noted in Llopis et al.
 337 [28], coplanar swimming is an unstable configuration. Figure 8 shows that
 338 even with symmetric motility patterns, fully three-dimensional trajectories
 339 may appear. We also see that these trajectories depend upon the intrinsic
 340 properties of the the actuated swimmer, since different planarity stiffness
 341 constants result in different trajectories. For the stiffness parameter values
 342 shown, it appears that a weaker planar restriction stiffness results in longer-
 343 term cooperativity, as the flagella remain close to each other for a longer
 344 period of time. This period of close swimming shows that symmetrically-
 345 beating sperm in different planes may move in wave-like patterns, weaving

346 around each other before eventually swimming away. Velocities for these
 347 swimmers decrease as they get closer to each other, but eventually increase
 348 towards that of a single swimmer as they swim apart (see Figure 6d). It
 349 appears that for transient periods of time, these swimmers may swim faster
 350 than a single swimmer due to their evolving relative orientation.

351 For a single flagellum, an asymmetric waveform acting upon a planar flag-
 352 ellum would result in a circular trajectory within the flagellar plane alone.
 353 Figure 9 shows that for two sperm, weak asymmetry in the waveform can lead
 354 to more complex three-dimensional trajectories. The flagellar plane of each
 355 individual sperm is rotated due to the presence of a nearby neighbor. Thus,
 356 spiral or pseudo-helical (“slinky”-like) trajectories can evolve from asymmet-
 357 ric waveforms. Movie M6 shows this swimming behavior over time. Movie
 358 M7 show high amplitude, strongly asymmetric waveforms that would charac-
 359 terize hyperactivity. Such high asymmetry and amplitude cause neighboring
 360 sperm to swim in more ball-like trajectories.

361 4. Conclusions

362 Mathematical and computational models have addressed various aspects
 363 of the hydrodynamic interaction of flagella, from infinite sheets [6, 13, 14,
 364 46] to more recent investigations in three dimensions [28, 29], along with
 365 novel laboratory experiments [5]. Here we have presented an extension of
 366 the driven elastica model of a swimming flagellum [17] into a fully three-
 367 dimensional formulation that penalizes out-of-plane waveforms. This allows
 368 the investigation of the fluid dynamic interaction of nearby swimmers, whose
 369 preferred planar waveforms may be altered by the flow.

370 This model is able to exhibit fully three-dimensional, helical and ball-like
 371 trajectories arising from simple planar waveforms due to fluid-structure cou-
 372 pling of nearby swimmers. In mammalian sperm, hyperactivity is thought to
 373 facilitate reorientation of the sperm body so that sperm can chemotactically
 374 move towards the egg [25]. The ball-like trajectories observed in our simu-
 375 lations of hyperactive waveforms may be functionally equivalent to the tum-
 376 bling state often described in bacterial chemotaxis, which enables bacteria
 377 to move towards favorable environments by randomly reorienting themselves
 378 before swimming in a new direction [2]. These trajectories, indeed, may be
 379 a benefit of complex environments and neighboring swimmers, in that they
 380 enable individual sperm to reorient in a fully three-dimensional space instead
 381 of just within their natural plane.

382 Cooperativity has been established in rodent sperm, where sperm cells
 383 swim together in the form of trains, but are also mechanically attached to
 384 each other by hook-like cell body structures [30]. In [40] we examined the
 385 hydrodynamics of sperm attachment and detachment from epithelia by al-
 386 lowing for forces due to dynamic elastic linkages between the actuated elastic
 387 flagellum and a planar wall. We will use the 3D extension described here,
 388 along with these dynamic linkages, to capture the complex binding interac-
 389 tions observed in some species [18, 24, 30, 31].

390 Our current model is a simplistic model chosen to compare with previ-
 391 ous planar model results. For instance, the effect of a sperm head has not
 392 been included in our model, which would introduce drag at the base of the
 393 flagellum and could affect motility patterns particularly near surfaces (see
 394 the recent work of Ishimoto and Gaffney [23]). Moreover, some species have

395 been shown experimentally to have three-dimensional sperm configurations
 396 that cannot be represented by simple planar forces described in our model.
 397 In fact, there is evidence that sperm flagella exhibit helical or non-planar
 398 waveforms in some settings [3, 36, 37, 51]. In Woolley and Osborn [50], the
 399 three-dimensional nature of hamster spermatozoa was determined to give
 400 rise to primarily clockwise torsional component, indicating that this came
 401 not from randomly applied (or external) forces but some structural feature
 402 of the flagellum itself. Additionally, the sea urchin behavior observed in some
 403 studies [10, 51] is thought to demonstrate a natural three-dimensional beat
 404 pattern which only reduces to a near-planar motion near surfaces. For these
 405 intrinsic three-dimensional waveforms, the method of regularized Stokeslets
 406 coupled to a Kirchhoff rod model [33] should be explored.

407 **5. Acknowledgements**

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410 **6. Conflict of interest statement**

411 The authors have no conflicts of interest to disclose.

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Parameter	Description	Value	Remark/Reference(s)
ϵ	Regularization parameter	$1.3 \mu\text{m}$	See [8]
	Diameter of sperm flagellum	$0.5 \mu\text{m}$	[38]
μ	Viscosity (water)	$10^{-3} \text{ kg m}^{-1} \text{ s}^{-1}$	
Δs	Spatial (arc length) discretization	$1 \mu\text{m}$	
L	Flagellum length	$100 \mu\text{m}$	[11]
b	Amplitude	$10 - 25 \mu\text{m}$	[32, 41]
κ	Wavenumber	$2\pi/L$	
ω	Frequency	20π (10 Hz)	[32, 41]
S_t	Tensile stiffness	$2 \text{ pN } \mu\text{m}^{-3}$	[40]
S_p	Planar restriction stiffness	$0.001 - 1 \text{ pN } \mu\text{m}^{-3}$	This work
S_b	Planar bending stiffness	$10 \text{ pN } \mu\text{m}^{-3}$	[34]
S_r	Repulsion stiffness	$5 \text{ aN } \mu\text{m}^{-3}$	This work
d	Repulsion length	$3 \mu\text{m}$	Set to be $> 2\delta$

Table 1: Parameter values used in models. Sperm parameters were set to that of a typical mammalian sperm (see [11]). The regularized delta function for the method of regularized Stokeslets is the same as in [34]. Note that in this framework, we are using force and energy densities, so stiffness constants include a factor of μm^{-3} .

550 8. Figures

551 **Figure 1:** Schematic of the physical domain of the discretized preferred
 552 configuration of the flagellum, with a sinusoidal waveform of amplitude b and
 553 an arc length along the flagellum ranging from $s = 0$ to $s = L$. Each point
 554 $\mathbf{X}_k$ experiences tensile forces from interactions with neighboring points, and
 555 bending forces that actuate the motion of the flagellum. The points have a
 556 preferred spacing of Δs .

557
 558 **Figure 2:** Example of a least squares fit plane to a flagellum given by
 559 data $\mathbf{X}_k$: (a) shows the original data, (b) shows the centered data with the
 560 least squares fit plane, and (c) shows the data in the flagellum frame of ref-
 561 erence with a least squares fit plane $\hat{z} = 0$. Dots represent the head of the
 562 sperm body, with darker shading showing the parts of the flagellum that are
 563 underneath the flagellar plane.

564
 565 **Figure 3:** Initial configurations of sperm flagella. In simulations with
 566 a single sperm, the black curve in (a)-(c) is used, and has a fully three-
 567 dimensional configuration. For two sperm coplanar simulations, we consider
 568 the flagella in panels (a)-(c), and project the black curve in (a)-(c) onto the
 569 plane $z = 0$ so both sperm are in the plane $z = 0$. For two sperm simulations
 570 with a non-planar perturbation, we use the red and black curves as shown in
 571 panels (a)-(c). For two sperm with initial parallel flagellar planes, we use the
 572 configurations in panels (d)-(f). All units are in μm . These small amplitude
 573 initial configurations are chosen for simplicity, and the sperm shape at later
 574 times is a sinusoidal form with an amplitude near $10 \mu\text{m}$, coming from the

575 energies defined in Section 2.1.

576

577 **Figure 4:** Comparison of maximal deviations from the flagellar plane
578 over time for various choices of planar restriction stiffness parameter S_p .
579 These deviations were calculated for a single sperm with the initial three-
580 dimensional configuration given by the black curve in Figure 3, using the
581 symmetric preferred curvature motility behavior.

582

583 **Figure 5:** Trajectories of the head points of two symmetrically beating
584 sperm with different planar initial conditions. Triangles represent final po-
585 sitions at time $t = 25$ s, and the starting position for the sperm heads is
586 at $x = 0$. Units are μm . Panel (a) initializes both flagella as coplanar in
587 the plane $z = 0$ with initial conditions corresponding to the projections of
588 the configurations in Figures 3a–3c onto $z = 0$. Panel (b) initializes both
589 flagella in parallel planes in y with initial conditions shown in Figures 3d–
590 3f. Note that coplanar flagella attract, whereas parallel planar flagella repel.
591 The Movies M2 and M3 show the swimming behavior of the trajectories in
592 (a) and (b), respectively, over time.

593

594 **Figure 6:** Average path velocities and minimum distance (magenta
595 curves) between flagella over time for symmetric swimmers with planar re-
596 striction stiffness $S_p = 1$. Panel (a) shows velocities from the initial parallel
597 configurations in Figure 3d–3f, corresponding to the trajectories in Figure 5b.
598 Panel (b) shows velocities from the same initial parallel configurations, ex-
599 cept the parallel planes are 10 times closer ($5 \mu\text{m}$ apart). To demonstrate at-

600 traction versus repelling swimming behavior, both parallel plane simulations
601 were run without any repulsion forces $\mathbf{g}_k^j$ that might interfere with trajec-
602 ries. Panel (c) shows velocities from the coplanar initial configurations given
603 by the projections of the configurations in Figure 3 onto the plane $z = 0$, cor-
604 responding to the trajectories in Figure 5a. Panel (d) shows velocities from
605 the non-planar initial configurations shown in Figure 3, corresponding to the
606 trajectories in Figure 8a. Both panels (c) and (d) show simulations run with
607 repulsion forces $\mathbf{g}_k^j$ present to prevent flagella from overlapping unrealistically.

608
609 **Figure 7:** Example of the positions of two symmetrically beating sperm
610 at $t = 0.1, 5.1$, and 10.1 seconds with planar restriction stiffness $S_p = 1$.
611 These are snapshots of sperm locations from the trajectories shown in Fig-
612 ure 8a. Units are μm . Initial configurations are shown in Figure 3. The
613 Movie M4 shows the swimming behavior of this simulation over time.

614
615 **Figure 8:** Example of trajectories of the head points of two symmetri-
616 cally beating sperm with different planar restriction stiffnesses S_p , over 25
617 seconds. Triangles represent final positions, starting position for sperm heads
618 is at $x = 0$. Units are μm . Initial configurations are shown in Figure 3. The
619 Movies M4 and M5 show the swimming behavior of the trajectories in (a)
620 and (b), respectively, over time.

621
622 **Figure 9:** Example of trajectories of the head points of weakly asym-
623 metrically beating sperm using a planar restriction stiffness of $S_p = 1$, traced
624 out over the times indicated with the initial configurations shown in Figures

625 3a-3c. “Zigzag” in the trajectories demonstrates the lateral displacement of
626 the head. Triangles (partially occluded) are placed at the end of trajectories,
627 starting position for sperm heads is at $x = 0$. Units are in μm . The Movies
628 M1 and M6 show the swimming behaviors of (a) and (b), respectively, over
629 time.

630

Figure 1: Schematic of the physical domain of the discretized preferred configuration of the flagellum, with a sinusoidal waveform of amplitude b and an arc length along the flagellum ranging from $s = 0$ to $s = L$. Each point $\mathbf{X}_k$ experiences tensile forces from interactions with neighboring points, and bending forces that actuate the motion of the flagellum. The points have a preferred spacing of Δs .

Figure 2: Example of a least squares fit plane to a flagellum given by data $\mathbf{X}_k$: (a) shows the original data, (b) shows the centered data with the least squares fit plane, and (c) shows the data in the flagellum frame of reference with a least squares fit plane $\hat{z} = 0$. Dots represent the head of the sperm body, with darker shading showing the parts of the flagellum that are underneath the flagellar plane.

Figure 3: Initial configurations of sperm flagella. In simulations with a single sperm, the black curve in (a)-(c) is used, and has a fully three-dimensional configuration. For two sperm coplanar simulations, we consider the flagella in panels (a)-(c), and project the black curve in (a)-(c) onto the plane $z = 0$ so both sperm are in the plane $z = 0$. For two sperm simulations with a non-planar perturbation, we use the red and black curves as shown in panels (a)-(c). For two sperm with initial parallel flagellar planes, we use the configurations in panels (d)-(f). All units are in μm . These small amplitude initial configurations are chosen for simplicity, and the sperm shape at later times is a sinusoidal form with an amplitude near $10 \mu\text{m}$, coming from the energies defined in Section 2.1.

Figure 4: Comparison of maximal deviations from the flagellar plane over time for various choices of planar restriction stiffness parameter S_p . These deviations were calculated for a single sperm with the initial three-dimensional configuration given by the black curve in Figure 3, using the symmetric preferred curvature motility behavior.

Figure 5: Trajectories of the head points of two symmetrically beating sperm with different planar initial conditions. Triangles represent final positions at time $t = 25$ s, and the starting position for the sperm heads is at $x = 0$. Units are μm . Panel (a) initializes both flagella as coplanar in the plane $z = 0$ with initial conditions corresponding to the projections of the configurations in Figures 3a–3c onto $z = 0$. Panel (b) initializes both flagella in parallel planes in y with initial conditions shown in Figures 3d–3f. Note that coplanar flagella attract, whereas parallel planar flagella repel. The Movies M2 and M3 show the swimming behavior of the trajectories in (a) and (b), respectively, over time.

Figure 6: Average path velocities and minimum distance (magenta curves) between flagella over time for symmetric swimmers with planar restriction stiffness $S_p = 1$. Panel (a) shows velocities from the initial parallel configurations in Figure 3d–3f, corresponding to the trajectories in Figure 5b. Panel (b) shows velocities from the same initial parallel configurations, except the parallel planes are 10 times closer (5 μm apart). To demonstrate attraction versus repelling swimming behavior, both parallel plane simulations were run without any repulsion forces $\mathbf{g}_k^j$ that might interfere with trajectories. Panel (c) shows velocities from the coplanar initial configurations given by the projections of the configurations in Figure 3 onto the plane $z = 0$, corresponding to the trajectories in Figure 5a. Panel (d) shows velocities from the non-planar initial configurations shown in Figure 3, corresponding to the trajectories in Figure 8a. Both panels (c) and (d) show simulations run with repulsion forces $\mathbf{g}_k^j$ present to prevent flagella from overlapping unrealistically.

Figure 7: Example of the positions of two symmetrically beating sperm at $t = 0.1, 5.1$, and 10.1 seconds with planar restriction stiffness $S_p = 1$. These are snapshots of sperm locations from the trajectories shown in Figure 8a. Units are μm . Initial configurations are shown in Figure 3. The Movie M4 shows the swimming behavior of this simulation over time.

Figure 8: Example of trajectories of the head points of two symmetrically beating sperm with different planar restriction stiffnesses S_p , over 25 seconds. Triangles represent final positions, starting position for sperm heads is at $x = 0$. Units are μm . Initial configurations are shown in Figure 3. The Movies M4 and M5 show the swimming behavior of the trajectories in (a) and (b), respectively, over time.

(a) Single sperm, $t = 0$ to 10 s.

(b) Two sperm, $t = 0$ to 25 s.

Figure 9: Example of trajectories of the head points of weakly asymmetrically beating sperm using a planar restriction stiffness of $S_p = 1$, traced out over the times indicated with the initial configurations shown in Figures 3a-3c. “Zigzag” in the trajectories demonstrates the lateral displacement of the head. Triangles (partially occluded) are placed at the end of trajectories, starting position for sperm heads is at $x = 0$. Units are in μm . The Movies M1 and M6 show the swimming behaviors of (a) and (b), respectively, over time.

631 9. Movie Legend

632 **Movie M1:** A weakly asymmetric swimmer starting with a perturbed
633 planar initial configuration (see black curve in Figures 3a–3c), with planar
634 stiffness constant $S_p = 1$. The sperm travels in a circular path, recovering
635 from its non-planar configuration quickly. Gray curve shows the projection
636 (“shadow”) of the flagellum on the plane $z = -100$. Units are in microns.
637 Length of simulation is 25 seconds.

638
639 **Movie M2:** Two symmetric swimmers with a coplanar initial config-
640 uration (see Figures 3a–3c), with planar stiffness constant $S_p = 1$. The
641 two swimmers attract over time. Light shaded curves show the projections
642 (“shadows”) of the flagella on the plane $z = -100$. Units are in microns.
643 Length of simulation is 25 seconds.

644
645 **Movie M3:** Two symmetric swimmers with a parallel planar initial con-
646 figuration (see Figures 3d–3f), with planar stiffness constant $S_p = 1$. The
647 two swimmers repel over time. Light shaded curves show the projections
648 (“shadows”) of the flagella on the plane $z = -100$. Units are in microns.
649 Length of simulation is 25 seconds.

650
651 **Movie M4:** Two symmetric swimmers with a perturbed planar initial
652 configuration (see Figures 3a–3c), with planar stiffness constant $S_p = 1$.
653 The two swimmers “weave” near each other before swimming apart. Light
654 shaded curves show the projections (“shadows”) of the flagella on the plane
655 $z = -150$. Units are in microns. Length of simulation is 25 seconds.

656

657   **Movie M5:** Two symmetric swimmers with a perturbed planar initial
658 configuration (see Figures 3a–3c), with planar stiffness constant $S_p = 0.01$.
659 The two swimmers “weave” near each other for a more prolonged period than
660 in Movie M4 because of a weaker stiffness constant. Light shaded curves show
661 the projections (“shadows”) of the flagella on the plane $z = -100$. Units are
662 in microns. Length of simulation is 25 seconds.

663

664   **Movie M6:** Two weakly asymmetric swimmers with a perturbed pla-
665 nar initial configuration (see Figures 3a–3c), with planar stiffness constant
666 $S_p = 1$. The two swimmers move in curved “slinky-like” trajectories over
667 time. Light shaded curves show the projections (“shadows”) of the flagella
668 on the plane $z = -250$. Units are in microns. Length of simulation is 25
669 seconds.

670

671   **Movie M7:** Two strongly asymmetric swimmers with a perturbed planar
672 initial configuration (see Figures 3a–3c), with planar stiffness constant $S_p =$
673 1. The two swimmers move in curved paths over time with a smaller radius of
674 curvature due to high asymmetry, resulting in “ball-like” trajectories. Light
675 shaded curves show the projections (“shadows”) of the flagella on the plane
676 $z = -100$. Units are in microns. Length of simulation is 25 seconds.