

A fully implicit method for robust frictional contact handling in elastic rods

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ABSTRACT

Accurate frictional contact is critical in simulating the assembly of rod-like structures in the practical world, such as knots, hairs, flagella, and more. Due to their high geometric nonlinearity and elasticity, rod-on-rod contact remains a challenging problem tackled by researchers in both computational mechanics and computer graphics. Typically, frictional contact is regarded as constraints for the equations of motions of a system. Such constraints are often computed independently at every time step in a dynamic simulation, thus slowing down the simulation and possibly introducing numerical convergence issues. This paper proposes a fully implicit penalty-based frictional contact method, Implicit Contact Model (IMC), that efficiently and robustly captures accurate frictional contact responses. We showcase our algorithm's performance in achieving visually realistic results for the challenging and novel contact scenario of flagella bundling in fluid medium, a significant phenomenon in biology that motivates novel engineering applications in soft robotics. In addition to this, we offer a side-by-side comparison with Incremental Potential Contact (IPC), a state-of-the-art contact handling algorithm. We show that IMC possesses comparable performance to IPC while converging at a faster rate.

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1. Introduction

Throughout human history, flexible filamentary structures have been essential to human society, serving various purposes such as fastening, sailing, climbing, weaving, and hunting. As our understanding of material properties improved, so did our ability to engineer rods with enhanced material properties (e.g., flexibility, strength, and resilience). This in turn has resulted in the need to study and better understand the complicated mechanics of filaments. Thus, several previous works have sought out to understand the various mechanics of rod-like structures including the deployment of rods [1–3], elastic gridshells [4–6], plant growth [7], knots [8–12], and propulsion of bacterial flagella [13–15].

With real-world experiments being costly and tedious to implement, the need for accurate physics-based numerical simulations is prevalent. Such simulations not only allow for advanced mechanics-based study, they also open up the avenue to challenging problems in robotics ranging from simulating soft robot

dynamics to closing the sim2real gap for deformable material manipulation. In recent times, discrete differential geometry-based (DDG-based) simulations have shown surprisingly successful performance in capturing the nonlinear mechanical behaviors of rod structures [16,17]. However, frictional contact handling still lacks a descriptive understanding.

Indeed, frictional contact formulations are usually diverse and based on the scaling of the system and/or the physical scenario. In this manuscript, we mainly focus on Coulomb friction, an adequate approximation of dry friction. Note that Coulomb friction degrades when contacted surfaces are conjoined. For engineering problems in which cohesion is important (e.g., cohesive granular media simulation [18–20]), a more elaborated contact theory such as Johnson-Kendall-Roberts (JKR), Derjaguin-Muller-Toporov (DMT), or Maugis models [21–23] are required. Some prior works use these elastic cohesive contact models to simulate incipient sliding of cohesive contacts [24,25]. Despite this, Coulomb friction is still the de facto friction model for non-cohesive contact due to its simplicity and high empirical accuracy, where it can be seen implemented in a wide variety of engineering applications, including, contact in elastic structures, most granular media simulations, and more. We therefore build a novel numerical framework based on Coulomb friction.

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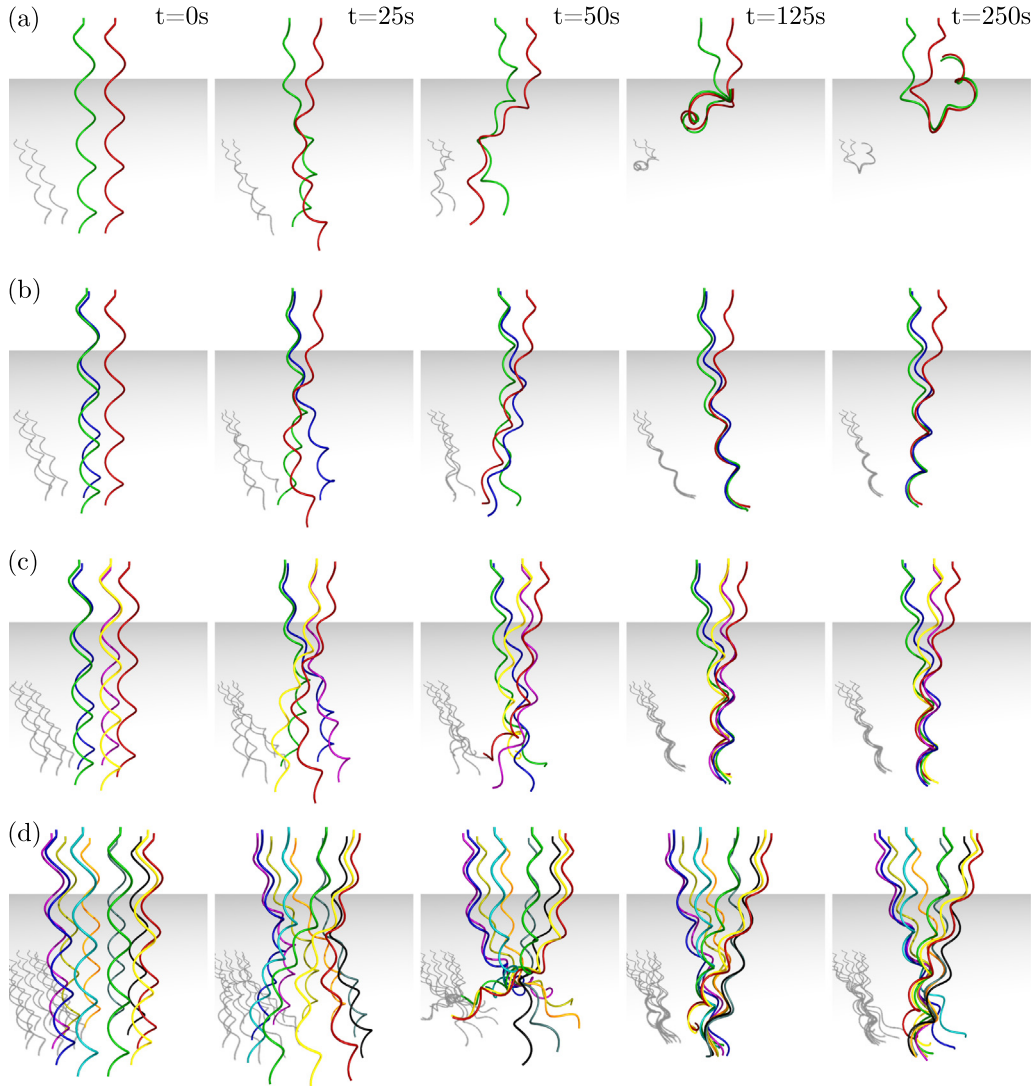


Fig. 1. Rendered snapshots of flagella bundling with varying amounts of flagella. Rows contain (a) $M = 2$, (b) $M = 3$, (c) $M = 5$, and (d) $M = 10$ flagella. Each column indicates the flagella configuration at the moment of time indicated in the top row.

Aside from friction formulations, contact handling methods can generally be divided into three distinct categories: impulse methods, constraint-based optimization methods, and penalty energy methods. As the name suggests, impulse methods compute contact forces based on the required impulse to keep rod segments from penetrating, with an example being the impulse force model by Spillmann et al. [26]. Although computationally efficient and straightforward to implement, unrealistic visual jittering often occurs when simulations use sufficiently large time steps as the generated forces are handled explicitly [27]. Therefore, impulse methods often must either deal with insufficient physical accuracy or use sufficiently small time steps.

Constraint-based methods treat frictional contact as a constrained optimization problem. Jean and Moreau [28,29] implemented convex analysis to propose using unilateral constraints to solve dry friction in granular media. Alart and Curnier [30] developed the first approach to solving constraint-based contact dynamics using Newton's method to find the root of a non-smooth function. In graphics, Daviet et al. [31] combined an analytical solver with the complementary condition from [30] to capture Coulomb friction in elastic fibers. In Ref. [32], the algorithm from [31] was incorporated with a nonlinear elasticity solver to simulate frictional contacts in assemblies of Discrete Elastic Rods [16,17]. Based on previous work, Daviet [33]

proposed a general constraint-based framework for simulating contact in thin nodal objects. Overall, constraint-based methods can often produce physically realistic results but are inherently more difficult to implement than impulse and penalty methods (though the growth of open source code has alleviated this considerably). Arguably the largest drawback of constraint-based methods, additional computational costs are incurred at each solving iteration as frictional contact forces must be introduced as additional degrees of freedom in order to satisfy the complementary condition between frictional contact responses and the status of contact regions. This is in contrast to impulse and penalty methods which can obtain contact responses directly based on just configuration-based degrees of freedom.

The final contact method type, penalty energy methods, utilize a formulated "contact energy" whose gradient is treated as the contact force. Due to the requirement of a smooth differentiable gradient (and Hessian for implicit formulations), such methods utilize smooth differentiable functions to best approximate the behavior of frictional contact [10,27,34]. These methods have become popular in recent times as they have been shown capable of generating accurate frictional contact [10,27] while remaining simple to implement (relative to constraint-based methods) and computationally efficient. Building upon this, we propose

Implicit Contact Model (IMC), a fully-implicit penalty-based contact model for frictional contact based on our previous work in Ref. [27]. We improve upon this iteration by (1) reformulating frictional contact to be fully-implicit for enhanced physical accuracy, (2) squaring our contact energy term for more rigid contact, (3) changing our smoothly approximated distance formulation to a more stable piecewise analytical formulation, and (4) adding a line search method for increased robustness. Our proposed numerical framework can generate contact for any rod-rod contact scenario and can also generate contact for 3D meshes with proper alterations.

In this paper, we choose to showcase our frictional contact model by simulating the novel and difficult contact scenario of flagella bundling [35–43], a significant natural phenomena that occurs when micro-organisms with multiple flagella swim in fluid (e.g., *Escherichia coli* and *Salmonella typhimurium* [44]). Each flagellum consists of a rotary “head”, a short flexible hook, and a helical filament. By rotating their filaments, these micro-organisms can navigate their environments through sophisticated manipulation of the solid–fluid interaction between their flexible structures and the surrounding flows. This has led to biomimicry, where flagella have inspired the design of several soft robot locomotion strategies in viscous fluids [45–49]. However, studying the mechanics of flagella is exceptionally challenging due to flagella possessing radii smaller than their optical wavelengths as well as having high rotational speeds [13].

This highlights the necessity for accurate simulators, the development of which is nontrivial due to the multifaceted problem of having to deal with hydrodynamic interactions, geometrically nonlinear deformations, and realistic contact handling. Prior works [37,41,42] usually consider the contact forces as simple repulsive forces. We instead incorporate our more principled frictional contact framework for the task of flagella bundling. Extensive validation of our generated frictional contact forces can be seen in Appendix C [50]. We note that despite this, our simulation results have not been validated for the task of flagella bundling in particular. Still, to the best of our knowledge, this paper is the first to design a fast and visually realistic simulator that can capture the bundling phenomena of multiple flagella rotating in low Reynolds number fluids. We believe our simulator has promise for aiding the study of flagella bundling where we conduct an informative parametric study for the bundling process using our framework in Appendix D [50]. It is also a first step towards efficient, physically realistic data generators for training bio-inspired flagellar robots for data-driven control approaches.

The primary contributions of our work are outlined below.

- We propose a fully-implicit penalty-based frictional contact model that has improved computational efficiency and accuracy compared with our previous work in Ref. [27].
- We formulate a full end-to-end framework for the novel and difficult contact scenario of flagella bundling in low Reynolds number fluids, which incorporates a DDG-based simulation framework, our frictional contact framework, and fluid–solid interaction.
- We conduct an in-depth side-by-side comparison between our proposed method (IMC) with the state-of-the-art (IPC) [34] and show that we are able to achieve faster convergence at the price of losing guarantee of non-penetration.
- We show visually convincing results for the sticking slipping phenomena of friction.

The remainder of the paper is as follows. In Section 2, we introduce the DDG-based framework for simulating a flexible rod. Next, in Section 3, we formulate our frictional contact model. Simulation results for IMC are then shown in Section 4 along with side-by-side comparisons with IPC and analysis of friction

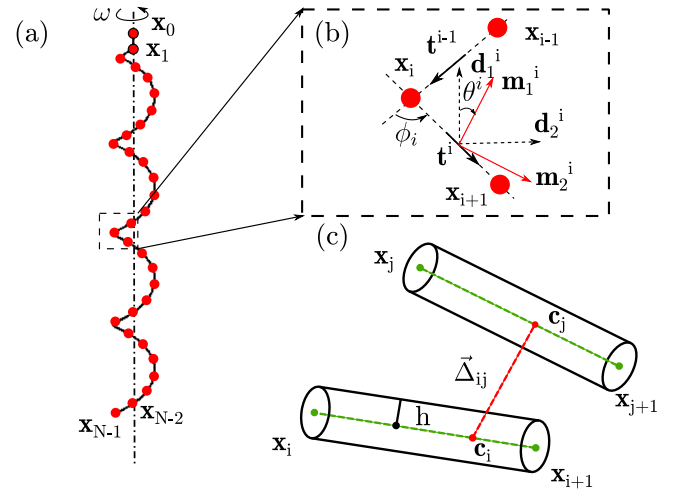


Fig. 2. (a) Discrete schematic of a flagellar elastic rod. Nodes $\mathbf{x}_0, \mathbf{x}_1$, and the edge between $\mathbf{x}_0$ and $\mathbf{x}_1$ is clamped along the dashed centerline and rotated with an angular velocity ω . The rest of the nodes constitute the helical flagellum which revolves around the centerline. (b) A zoomed in snapshot of two edges showcasing their reference frame, material frame, turning angles, and twist angles. (c) Illustration of two edges approaching contact. The green dots showcase the nodes of the edges while the green dashed lines denote the centerlines of the edges. The red dashed line denotes the vector $\vec{\Delta}$ whose norm is the minimum distance Δ between the edges. Δ is connected to edges i and j by $\mathbf{c}_i = \mathbf{x}_i + \beta_i(\mathbf{x}_{i+1} - \mathbf{x}_i)$ and $\mathbf{c}_j = \mathbf{x}_j + \beta_j(\mathbf{x}_{j+1} - \mathbf{x}_j)$ where $\beta_i, \beta_j \in [0, 1]$. As Δ approaches the contact threshold $2h$, repulsive forces increase at an exponential rate, thus enforcing non-penetration. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

performance. Finally, in Section 5, we provide concluding remarks as well as potential future research directions. Further details on the fluid–solid interaction model, IMC algorithmic components, and miscellaneous information can be found in Supplementary Information Appendices A, B, and E, respectively [50]. All source code used in this paper is released publicly and can be found at <https://github.com/StructuresComp/rod-contact-sim>.

2. Discrete elastic rods

In order to simulate the geometric nonlinear behaviors of flagella in viscous fluids, we utilize the DDG-based framework Discrete Elastic Rods (DER) [16,17]. As shown in Fig. 2(a), DER expresses the centerline of an elastic rod with N discrete nodes: $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_{N-2}, \mathbf{x}_{N-1}$. This results in a total of $N - 1$ edges where $\mathbf{e}^i = \mathbf{x}_{i+1} - \mathbf{x}_i$. Note that for DER, we use subscripts to denote indices for quantities associated with nodes and superscripts for indices for quantities associated with edges. Following this, each edge $\mathbf{e}^i$ is described using two orthogonal frames: a reference frame $\{\mathbf{t}^i, \mathbf{d}_1^i, \mathbf{d}_2^i\}$ and a material frame $\{\mathbf{t}^i, \mathbf{m}_1^i, \mathbf{m}_2^i\}$ as shown in Fig. 2(b). The reference frame is predefined at initial time $t = 0s$. The material frame shares the same director $\mathbf{t}^i = \mathbf{e}^i / \|\mathbf{e}^i\|$ as the reference frame and is obtainable through a twist angle θ^i with respect to the reference frame. A total of N nodes, each represented by a Cartesian coordinate $\mathbf{x}_i \in \mathbb{R}^3$, and $N - 1$ twist angles constitute a total of $4N - 1$ degrees of freedom: $\mathbf{q} = [\mathbf{x}_0, \theta^0, \mathbf{x}_1, \dots, \mathbf{x}_{N-2}, \theta^{N-2}, \mathbf{x}_{N-1}]$.

To simulate the elastic properties of a rod, we must compute elastic energies as defined by strain. Based off of Kirchhoff's rod model [51], strains can be divided into three categories: stretching, bending, and twisting. Starting off, the stretching strain of an edge $\mathbf{e}^i$ is described by

$$\epsilon^i = \frac{\|\mathbf{e}^i\|}{\|\bar{\mathbf{e}}^i\|} - 1, \quad (1)$$

where $\|\bar{\mathbf{e}}^i\|$ is the undeformed length of edge $\mathbf{e}^i$. From hereafter, quantities with a $\bar{}$ represent their values in their undeformed state.

Moving forwards, the bending strain for a node $\mathbf{x}_i$ is evaluated by a curvature binormal which captures the misalignment between two consecutive edges:

$$(\kappa \mathbf{b})_i = \frac{2\mathbf{e}^{i-1} \times \mathbf{e}^i}{\|\mathbf{e}^{i-1}\| \|\mathbf{e}^i\| + \mathbf{e}^{i-1} \cdot \mathbf{e}^i}. \quad (2)$$

Here, $\|(\kappa \mathbf{b})_i\| = 2 \tan(\phi_i/2)$, where ϕ_i is the turning angle shown in Fig. 2(b). The material curvatures are the components of the curvature binormal $(\kappa \mathbf{b})_i$ via the directors of the material frame:

$$\begin{aligned} \kappa_i^{(1)} &= \frac{1}{2}(\mathbf{m}_2^{i-1} + \mathbf{m}_2^i) \cdot (\kappa \mathbf{b})_i, \\ \kappa_i^{(2)} &= \frac{1}{2}(\mathbf{m}_1^{i-1} + \mathbf{m}_1^i) \cdot (\kappa \mathbf{b})_i. \end{aligned} \quad (3)$$

Finally, the twisting strain for a node $\mathbf{x}_i$ is computed as

$$\tau_i = \theta^i - \theta^{i-1} + m_{\text{ref}}^i, \quad (4)$$

where m_{ref}^i is the difference between the two consecutive reference frames of the i and $i-1$ -th edges.

With all strains defined, we can now formulate the stretching, bending, and twisting energy of a discretized elastic rod:

$$\begin{aligned} E_s &= \frac{1}{2} \sum_{i=0}^N EA(\epsilon^i)^2 \|\bar{\mathbf{e}}^i\|, \\ E_b &= \frac{1}{2} \sum_{i=1}^N \frac{1}{\Delta l_i} \left[EI_1 \left(\kappa_i^{(1)} - \bar{\kappa}_i^{(1)} \right)^2 + EI_2 \left(\kappa_i^{(2)} - \bar{\kappa}_i^{(2)} \right)^2 \right], \\ E_t &= \frac{1}{2} \sum_{i=1}^N \frac{GJ}{\Delta l_i} (\tau_i)^2, \end{aligned} \quad (5)$$

where E is Young's Modulus; A is the cross-sectional area; G is the shear modulus; J is the polar second moment of area along tangent $\mathbf{t}^i$; I_1 and I_2 are moments of inertia along material directors $\mathbf{m}_1^i$ and $\mathbf{m}_2^i$; and $\Delta l_i = (\|\mathbf{e}^i\| + \|\mathbf{e}^{i+1}\|)/2$ is the Voronoi length.

Next, the internal forces (for each nodal degree of freedom) and moments (for each twist degree of freedom) can be obtained via the partial derivative of the sum of elastic energies given in Eq. (5) as shown:

$$\mathbf{F}_i^{\text{int}} = - \frac{\partial(E_s + E_b + E_t)}{\partial \mathbf{q}_i} \quad \forall i \in [0, 4N-1]. \quad (6)$$

These quantities result in a $4N-1$ sized force vector $\mathbf{F}^{\text{int}}$. Following this, we can write the system of equations of motions as the sum of inertial terms, internal forces, and external forces (e.g. contact, friction, gravity). This results in the equation

$$\mathbf{F} \equiv \mathbb{M} \ddot{\mathbf{q}} - \mathbf{F}^{\text{int}} - \mathbf{F}^{\text{ext}} = \mathbf{0}, \quad (7)$$

where $\mathbb{M}$ is the diagonal mass matrix, $\ddot{\mathbf{q}}$ is the second derivative of the DOFs with respect to time, $\mathbf{F}^{\text{ext}}$ is the external force vector, and $\mathbf{F}$ is the total force. This external force vector will be made up of our contact forces described in Section 3 as well as viscous drag forces from solid-fluid interactions described in Supplementary Information [50]. As Eq. (7) is a root-finding problem, we use Newton's method to solve the system of equations to march through time. Note that the Jacobian of the viscous drag forces is unobtainable. Therefore, viscous drag forces are treated explicitly, i.e. their Jacobian is simply ignored. Still, as our contact model is fully implicit, we are able to robustly simulate flagella bundling regardless of the explicitly added forces, as we will soon show.

3. Contact model methodology

Moving forwards, we denote the following vector concatenation describing an edge-to-edge contact pair: $\mathbf{x}_{ij} := (\mathbf{x}_i, \mathbf{x}_{i+1}, \mathbf{x}_j, \mathbf{x}_{j+1}) \in \mathbb{R}^{12}$, where $|j-i| > 1$ to exclude consecutive edges from consideration when enforcing contact. We describe the set of all valid edge combinations as $\mathcal{X}$. In future equations, we simply denote the subscriptless $\mathbf{x}$ as an arbitrary edge combination for clarity. We design a contact energy $E(\Delta(\mathbf{x}))$ to increase as the minimum distance Δ between two bodies approaches a contact threshold ($2h$ for our application where h is the radius of the flagella). With this, the contact energy gradient $-k \nabla_{\mathbf{x}} E(\mathbf{x}) \in \mathbb{R}^{12}$ is used as the contact forces while the contact energy Hessian $-k \nabla_{\mathbf{x}}^2 E(\mathbf{x}) \in \mathbb{R}^{12 \times 12}$ is used as the contact force Jacobian, where k is the contact stiffness which scales the contact forces appropriately to enforce non-penetration. In the upcoming sections, we will now formulate contact energy $E(\Delta(\mathbf{x}))$, minimum distance between two edges $\Delta(\mathbf{x})$, as well as friction.

3.1. Contact energy

In the ideal setting, contact energy must satisfy two properties: (1) it is zero for any distance $\Delta > 2h$ and (2) it is non-zero at exactly distance $\Delta = 2h$. A Heaviside step function can essentially describe these properties. Such a function is non-smooth with a very sudden discontinuous change in value, and therefore, cannot be solved reliably by root-finding algorithms such as Newton's method. To remedy this, IPC uses the following energy formulation to smoothly approximate contact:

$$E^{\text{IPC}}(\Delta, \delta) = \begin{cases} -(\Delta - (2h + \delta))^2 \ln\left(\frac{\Delta}{2h + \delta}\right), & \Delta \in (2h, 2h + \delta) \\ 0 & \Delta \geq 2h + \delta, \end{cases} \quad (8)$$

where δ is the distance tolerance that defines the region $(2h, 2h + \delta)$ for which non-zero forces are experienced. This contact energy approaches ∞ when Δ decreasingly approaches $2h$ and is therefore undefined for the region $\Delta \leq 2h$. Although this barrier formulation allows IPC to strictly enforce non-penetration, the solver must be careful never to allow any contact pairs in the penetration zone and/or venture into this undefined region during the optimization process. This is ensured by the inclusion of a custom line search method which conservatively sets an upper bound for the Newton update coefficient α .

In contrast to this, we design our energy formulation to allow for optimization into the penetrated region, thus expanding the range contact forces are experienced from $\Delta \in (2h, 2h + \delta)$ to $\Delta \in (0, 2h + \delta)$. This in turn allows us to take advantage of more aggressive line search methods, which leads to faster convergence for the flagella contact problem. Although this in theory allows our model to be susceptible to penetration, a sufficient contact stiffness k remedies this issue. We provide a method that adaptively sets an appropriate stiffness value in Supplementary Information [50]. In addition, to further ensure non-penetration, we take our previous energy formulation from [27] and square it so that our gradient grows exponentially instead of linearly. In the end, we use the smooth approximation

$$E(\Delta, \delta) = \begin{cases} (2h - \Delta)^2 & \Delta \in (0, 2h - \delta) \\ \left(\frac{1}{K_1} \log(1 + \exp(K_1(2h - \Delta))) \right)^2 & \Delta \in (2h - \delta, 2h + \delta) \\ 0 & \Delta \geq 2h + \delta, \end{cases} \quad (9)$$

where $K_1 = 15/\delta$ indicates the stiffness of the energy curve.

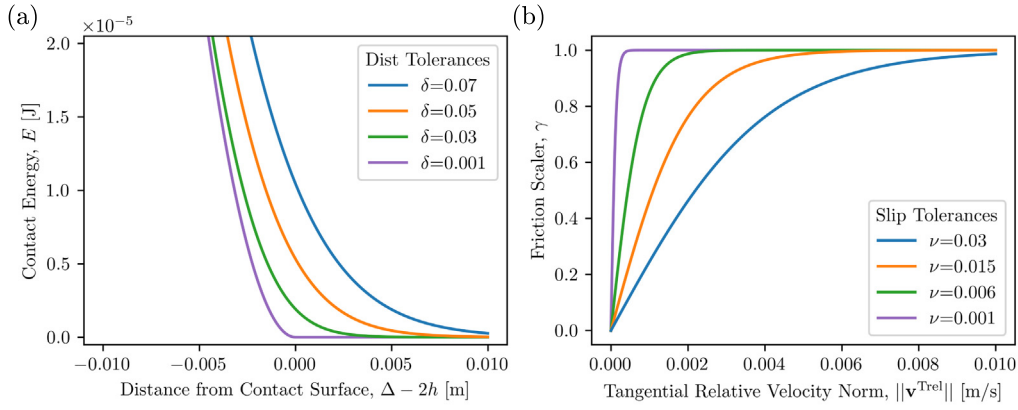


Fig. 3. Plots for the approximation functions in (a) Eq. (9) and (b) Eq. (17) with varying tolerance values. Note that some of the tolerances displayed are unrealistically large for clarity.

We incorporate the piecewise term $(2h - \Delta)^2$ for two reasons. First, this term equivalently models our energy formulation for the region $\Delta \leq 2h - \delta$ and has a simpler gradient and Hessian, resulting in computational efficiency. Second, and more importantly, the piecewise term also ensures numeric stability by preventing the exponential term in Eq. (9) from exploding. We show our plotted energy term in Fig. 3(a) for various δ values. As shown, the energy starts to increase at an exponential rate as Δ decreases towards the contact limit which is shown as 0 here. As δ decreases, more realistic contact is achieved (enhancing accuracy) in exchange for a stiffer equation (more difficult to converge).

3.2. Computing distance

As mentioned in [34], the minimum distance between two edges $(\mathbf{x}_i, \mathbf{x}_{i+1})$ and $(\mathbf{x}_j, \mathbf{x}_{j+1})$ can be formulated as the constrained optimization problem

$$\Delta = \min_{\beta_i, \beta_j} \|\mathbf{x}_i + \beta_i(\mathbf{x}_{i+1} - \mathbf{x}_i) - (\mathbf{x}_j + \beta_j(\mathbf{x}_{j+1} - \mathbf{x}_j))\| \ni 0 \leq \beta_i, \beta_j \leq 1, \quad (10)$$

where β_i and β_j represent the contact point ratios along the respective edges. Minimum distance between two edges can be classified into three distinct categories: point-to-point, point-to-edge, and edge-to-edge. As the names suggest, these classifications depend on which points of the edges the minimum distance vector Δ lies as described by β_i and β_j shown in Fig. 2(c).

In our previous work [27], we altered Lumelsky's edge-to-edge minimum distance algorithm [52] (which implicitly computes the β values) to be fully differentiable through smooth approximations. In this work, we now change the distance formulation to use piecewise analytical functions as shown below in Eq. (11), (12), and (13), similar to [34], as we found more stable performance compared to our smooth formulation despite the non-smooth Hessian when changing between contact categories.

We now describe the conditions for each contact type classification. First, if Δ lies on the ends of both edges (i.e. both β constraints are active), then the distance formulation degenerates to the point-to-point case which can easily be solved using the Euclidean distance formula,

$$\Delta^{PP} = \|\mathbf{x}_a - \mathbf{x}_b\|, \quad (11)$$

where $\mathbf{x}_a$ and $\mathbf{x}_b$ are the nodes for first and second edges in contact, respectively.

Algorithm 1: Implicit Contact Model

Input: $\mathbf{x}, \mathbf{x}_0, k, \delta, \nu$

Output: $\mathbf{F}^c, \mathbf{J}^c, \mathbf{F}^{fr}, \mathbf{J}^{fr}$

```

1 Function IMC( $\mathbf{x}, \mathbf{x}_0, k, \delta, \nu$ ):
2    $\mathbf{v} \leftarrow \mathbf{x} - \mathbf{x}_0$  // compute velocity
3    $\mathbf{F}^c, \mathbf{J}^c \leftarrow \text{genContact}(\mathbf{x}, \delta)$  // Eq. (9)
4    $\mathbf{F}^c \leftarrow k\mathbf{F}^c$  // scale by contact stiffness
5    $\mathbf{J}^c \leftarrow k\mathbf{J}^c$  //  $\mathbf{J}^c \equiv \nabla_{\mathbf{x}}\mathbf{F}^c$ 
6    $\mathbf{F}^{fr} \leftarrow \text{genFriction}(\mathbf{x}, \mathbf{v}, \mathbf{F}^c, \nu)$  // Eq. (18)
7    $\nabla_{\mathbf{x}}f, \nabla_{\mathbf{v}}f \leftarrow \text{genFrictionPartials}(\mathbf{x}, \mathbf{v}, \mathbf{F}^c, \nu)$ 
   //  $\mathbf{F}^{fr} \equiv f(\mathbf{x}, \mathbf{F}^c)$ 
8    $\mathbf{J}^{fr} \leftarrow \nabla_{\mathbf{x}}f + \nabla_{\mathbf{v}}f \nabla_{\mathbf{x}}\mathbf{F}^c$  // Eq. (21)
9   return  $\mathbf{F}^c, \mathbf{J}^c, \mathbf{F}^{fr}, \mathbf{J}^{fr}$ 

```

If Δ only lies on one end of one rod (i.e. only one β constraint is active), then the contact type degenerates to point-to-edge. This can be solved as

$$\Delta^{PE} = \frac{\|(\mathbf{x}_a - \mathbf{x}_b) \times (\mathbf{x}_b - \mathbf{x}_c)\|}{\|\mathbf{x}_a - \mathbf{x}_b\|}, \quad (12)$$

where $\mathbf{x}_a$ and $\mathbf{x}_b$ are the nodes of the edge for which the minimum distance vector does not lie on an end and $\mathbf{x}_c$ is the node of the edge which the minimum distance vector does lie on. Finally, edge-to-edge distance (i.e. no active constraints) for the i th and j th edges can be solved as

$$\begin{aligned} \mathbf{u} &= (\mathbf{x}_{i+1} - \mathbf{x}_i) \times (\mathbf{x}_{j+1} - \mathbf{x}_j), \\ \Delta^{EE} &= |(\mathbf{x}_i - \mathbf{x}_j) \cdot \hat{\mathbf{u}}|, \end{aligned} \quad (13)$$

where $\hat{\mathbf{u}}$ indicates a unit vector. With Δ fully defined, this concludes our contact energy formulation. To correctly classify contact pairs, we use Lumelsky's algorithm to compute β values.

3.3. Adding friction

Similar to before, we model friction according to Coulomb's friction law, which describes the conditions necessary for two solids to transition between sticking and sliding. This law states that the frictional force $\mathbf{F}^{fr}$ is (1) equal to $\mu\mathbf{F}^n$ during sliding, (2) is in the region of $[0, \mu\mathbf{F}^n]$ when sticking, and (3) is independent of the magnitude of velocity. Here, μ is the friction coefficient and $\mathbf{F}^n$ is the normal force experienced by the body.

Let us denote the following equivalencies for clarity: $\mathbf{F}^c \equiv k\nabla_{\mathbf{x}}E$ and $\mathbf{J}^c \equiv k\nabla_{\mathbf{x}}^2E$. Following this, for a contact pair $\mathbf{x}_{ij} := (\mathbf{x}_i, \mathbf{x}_{i+1}, \mathbf{x}_j, \mathbf{x}_{j+1})$, we can obtain the normal force on the i th and

$i + 1$ -th nodes as $F_i^n = \|F_i^c\|$ and $F_{i+1}^n = \|F_{i+1}^c\|$, respectively. This in turn allows us to obtain the contact norm vector

$$\mathbf{n}_i = \frac{\mathbf{F}_i^c + \mathbf{F}_{i+1}^c}{\|\mathbf{F}_i^c + \mathbf{F}_{i+1}^c\|}. \quad (14)$$

The direction of friction is then the tangential relative velocity between edges i and j . To compute this, we must first compute the relative velocities of the edges at the point of contact, which can be done using $\beta_i, \beta_j \in [0, 1]$ as shown below:

$$\begin{aligned} \mathbf{v}_i^e &= (1 - \beta_i)\mathbf{v}_i + \beta_i\mathbf{v}_{i+1}, \\ \mathbf{v}_j^e &= (1 - \beta_j)\mathbf{v}_j + \beta_j\mathbf{v}_{j+1}, \\ \mathbf{v}^{\text{rel}} &= \mathbf{v}_i^e - \mathbf{v}_j^e, \end{aligned} \quad (15)$$

where $\mathbf{v}_i, \mathbf{v}_{i+1}, \mathbf{v}_j$, and $\mathbf{v}_{j+1}$ are the velocities of the i th, $i + 1$ -th, j th, and $j + 1$ -th nodes, respectively. The tangential relative velocity of edge i with respect to edge j can then be computed as

$$\mathbf{v}^{\text{Trel}} = \mathbf{v}^{\text{rel}} - (\mathbf{v}^{\text{rel}} \cdot \mathbf{n}_i)\mathbf{n}_i, \quad (16)$$

where $\hat{\mathbf{v}}^{\text{Trel}} = \mathbf{v}^{\text{Trel}} / \|\mathbf{v}^{\text{Trel}}\|$ is our friction direction.

Now, we must also make our contact model capable of simulating the transition between sticking and sliding. Coulomb's law tells us that $\|\mathbf{v}^{\text{Trel}}\| = 0$ during static friction and that $\|\mathbf{v}^{\text{Trel}}\| > 0$ for sliding friction. Sticking occurs up until the tangential force threshold μF^n is surpassed, after which sliding begins. This relation (similar to ideal contact energy) can also be described by a modified Heaviside step function. For the same reasons as before, we replace this step function for another smooth approximation described by

$$\gamma(\|\mathbf{v}^{\text{Trel}}\|, \nu) = \frac{2}{1 + \exp(-K_2\|\mathbf{v}^{\text{Trel}}\|)} - 1, \quad (17)$$

where ν (m/s) is our desired slipping tolerance and $K_2(\nu) = 15/\nu$ is the stiffness parameter. As shown in Fig. 3(b), $\gamma \in [0, 1]$ smoothly scales the friction force magnitude from zero to one as $\|\mathbf{v}^{\text{Trel}}\|$ increases from zero. The slipping tolerance describes the range of velocities $(0, \nu)$ for which a friction force $< \mu F^n$ is experienced. In other words, we consider velocities within this range to be "sticking".

Finally, the friction experienced by a node i for a contact pair $\mathbf{x}_{ij}$ can be described as

$$\mathbf{F}_i^{\text{fr}} = -\mu\gamma\hat{\mathbf{v}}^{\text{Trel}}F_i^n. \quad (18)$$

With friction fully defined, we can now formulate the friction Jacobian $\nabla_{\mathbf{x}}\mathbf{F}^{\text{fr}}$. Note that due to Eq. (15), our formulation depends on $\beta(\mathbf{x})$, which means that the gradient $\nabla_{\mathbf{x}}\beta$ is required. We can avoid this computation through the realization that the magnitudes of the contact forces $\mathbf{F}_i^c$ and $\mathbf{F}_{i+1}^c$ have an underlying linear relationship with β where

$$\begin{aligned} \mathbf{F}_i^c &= (1 - \beta)(\mathbf{F}_i^c + \mathbf{F}_{i+1}^c), \\ \mathbf{F}_{i+1}^c &= \beta(\mathbf{F}_i^c + \mathbf{F}_{i+1}^c). \end{aligned} \quad (19)$$

Therefore, we can obtain β by simply solving

$$\beta = \frac{\|\mathbf{F}_{i+1}^c\|}{\|\mathbf{F}_i^c + \mathbf{F}_{i+1}^c\|}. \quad (20)$$

We can now treat β as a function of $\mathbf{F}^c$, resulting in a simplified chain ruling procedure. Let us denote Eq. (18) as the functional $f(\mathbf{x}, \mathbf{F}^c(\mathbf{x}))$. The friction Jacobian can then be computed through chain rule as

$$\nabla_{\mathbf{x}}\mathbf{F}^{\text{fr}} = \nabla_{\mathbf{x}}f + \nabla_{\mathbf{F}^c}f\nabla_{\mathbf{x}}\mathbf{F}^c. \quad (21)$$

This concludes our fully implicit friction scheme. Full pseudocode for the IMC algorithm can be found in Algorithm 1.

4. Simulation results

In this section, we showcase extensive quantitative and qualitative results for IMC. First, we discuss all our simulation parameters. We then conduct a detailed comparison between IMC and the state-of-the-art contact handling method: Incremental Potential Contact (IPC) [34]. Afterwards, we showcase comprehensive results concerning friction and display IMC's ability to simulate the sticking sliding transition.

4.1. Parameters and setup

In the simulation, we design the flagella as right-handed helical rods manufactured with linear elastic material. We set the material properties as follows: Young's modulus was set to $E = 3.00$ MPa; Poisson's ratio was set to 0.5; density of the rod was set to $\rho = 1000$ kg/m³; the cross-sectional radius was set to $h = 1$ mm, and the fluid viscosity was set to 0.1 Pa·s. Here, a Poisson's ratio of 0.5 was chosen to enforce the flagella to be an incompressible material. The topologies of the flagella are helices with helical radius $a = 0.01$ m, helical pitch $\lambda = 0.05$ m, and axial length $z_0 = 0.2$ m. These parameters were chosen as they best mimic the geometries of biological flagella found in nature [13,15,42,53].

We explore the bundling phenomena with M flagella ($M = [2, 3, 5, 10]$) where the rotating ends of each flagella is fixed along the z -axis as shown in Fig. 2(a). These rotating ends are treated as boundary conditions and are spaced out equidistantly so as to form a regular polygon with M angles with side length $\Delta L = 0.03$ m as shown in Fig. 4(c). We set the rotation speed of the flagella ends to $\omega = 15$ rad/s which keeps the Reynolds number in our numerical simulation to be always smaller than 4×10^{-2} , thus satisfying the Stokes flow.

Finally, we discretize each flagella into 68 nodes for a total of 67 edges. We found this discretization to have the best trade-off between computational efficiency and accuracy. Furthermore, we set the time step size to $\Delta t = 1$ ms. As the forces generated from our fluid model are handled explicitly, we found 1 ms to be the largest stable time step size before convergence performance became hampered. A distance tolerance of $\delta = 1 \times 10^{-5}$ was used for all simulations.

4.2. Comparison between IMC and IPC

Both IMC and IPC were used to simulate 250 s of rotation for scenarios with 2, 3, 5, and 10 flagella as shown in Fig. 1. As the friction coefficient between structures is usually trivial in viscous fluids, we consider purely contact without friction ($\mu = 0$). First, a side-by-side visual comparison for $M = 5$ is shown for IMC and IPC in Fig. 4(a). For various time steps, we can see that the configurations of the flagella are near identical, indicating that both methods have comparable performance. To further study this similarity, we define normalized average difference $\bar{e}$ to measure the difference in flagella nodal configurations between IMC and IPC:

$$\bar{e} = \frac{1}{MNh} \sum_{i=0}^{M-1} \sum_{j=0}^{N-1} \|\mathbf{x}_j^{i,\text{IMC}} - \mathbf{x}_j^{i,\text{IPC}}\|, \quad (22)$$

The relationship between normalized average difference $\bar{e}$ and time t is shown in Fig. 4(d). Here, we can find that the difference between the configurations is quite minimal, further cementing the notion that IMC has comparable performance to IPC despite the loss of non-penetration guarantee.

Where IMC starts to improve upon IPC is in terms of computational efficiency. Detailed metrics for all runs can be seen

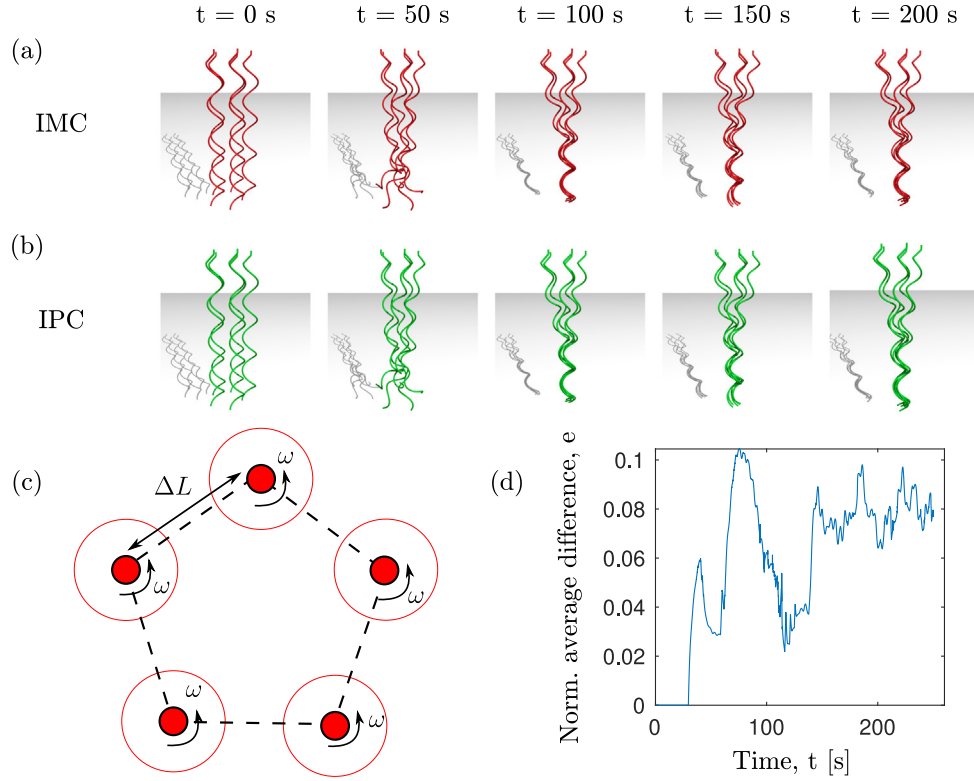


Fig. 4. Rendered snapshots for $M = 5$ flagella simulated by (a) IMC and (b) IPC. We can observe that there is great qualitative agreement between both methods at the shown time steps. (c) A top down visualization of boundary conditions applied to the highest nodes (filled in red circles) of each flagella as well as the angular rotation ω applied to them. The larger hollow red circles represent the rest of the helical flagella. (d) The norm of the average difference in the nodal positions for the flagella simulated by IMC and IPC with respect to time. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 1

IMC vs. IPC [34] run time data. Simulations are run for a total of 250 s with a time step size of $\Delta t = 1$ ms and a rotation speed of $\omega = 15$ rad/s. The contact model used can be seen in the far left column. Next to this, M indicates the number of flagella. AIPTS stands for average iterations per time step. ATPTS stands for average time per time step. Total Iters indicates the total number of Newton's iterations that were necessary to complete the simulation. The Total Run Time is the total computational time to completion. Finally, RTI stands for run time improvement and is the ratio of improvement between IMC's and IPC's total run time.

Model	M	AIPTS	ATPTS [ms]	Total Iters	Total Run Time [h]	RTI
IMC	2	3.00	10.2	6.01×10^5	0.57	1.82
	3	3.01	21.3	6.04×10^5	1.19	1.82
	5	3.02	67.5	5.39×10^5	3.34	1.40
	10	3.12	389.4	6.56×10^5	22.77	1.22
IPC	2	4.00	18.75	7.98×10^5	1.04	N/A
	3	4.00	39.5	7.93×10^5	2.17	N/A
	5	4.01	95.3	7.09×10^5	4.68	N/A
	10	4.02	477.47	8.45×10^5	27.88	N/A

in Table 1 which showcase the average iteration per time step (AIPTS), average time per time step (ATPTS), total iterations, and total run time. All metrics were recorded using time steps with at least one contact. Here, we can see that IMC was able to converge with less average iterations than IPC for all flagella cases resulting in significant reductions in total run time. These run time improvements are most drastic for $M = 2$ and $M = 3$ and start to decrease as M increases further as the RSS force computation starts to become a bottleneck. Regardless, a clear monotonic decrease can still be seen.

4.3. Friction example

Although friction is usually negligible in a viscous fluid medium, influence of friction on flagella bundling is still intriguing since the effect of friction can become significant as

the environment changes (e.g., granular medium). We assume an imaginary viscous environment where the friction coefficient between structures is non-negligible. We present simulation data for two flagella ($M = 2$) with friction coefficients $\mu = [0.1, 0.2, \dots, 1.0]$. For all simulations, a slipping tolerance of $\nu = 1 \times 10^{-4}$ was used. All other parameters are kept the same as before.

We first showcase the sticking slipping phenomena with snapshots for $\mu = [0, 0.3, 0.7]$ in Fig. 5. Intuitively, as μ increases, we also see the amount of sticking increase as well. Convergence results for all friction examples can be seen in Table 2 where average iterations per time step and simulation length are reported. Here, we notice two trends. First, for $\mu \geq 0.7$, the time at which the simulation ends starts to decrease from 250 s. This is because $\mu = 0.7$ is the point at which the flagella become completely tangled as shown in the bottom right frame of Fig. 5.

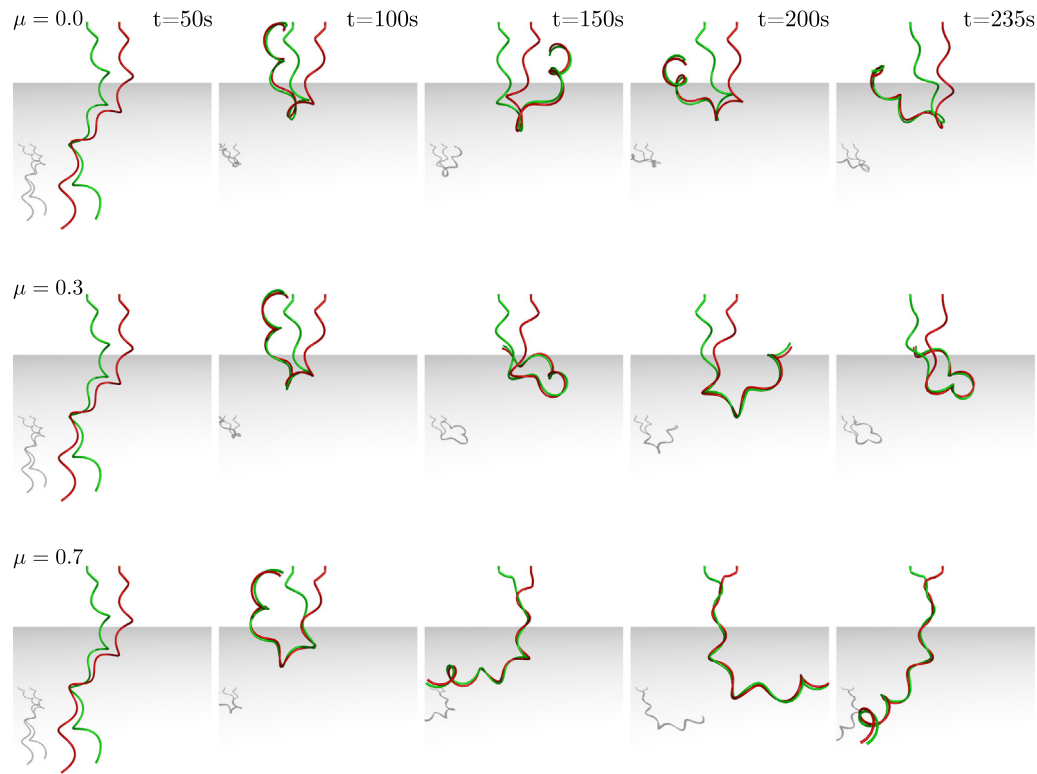


Fig. 5. Rendered snapshots for $M = 2$ with varying friction coefficients. Each column indicates a moment in time as indicated by the time stamp in the top row. The first row shows the frictionless case $\mu = 0$ as a baseline. The second row has $\mu = 0.3$ where minor sticking can be observed as the point at where the flagella no longer contact is higher than the frictionless case. Still, $\mu = 0.3$ still has plenty of slipping allowing the flagella to not become coiled. As we increase μ to 0.7 in the third row, we can see the amount of sticking increase, ultimately resulting in the flagella becoming completely coiled.

Table 2

Friction results for varying friction coefficients. AIPTS stands for average iterations per time step. Total Iterations indicate the total number of Newton's method iterations that were necessary to complete the simulation. Sim End indicates the total simulated time. All simulations were set to run for 250 s. As can be seen, simulations with $\mu \geq 0.7$ end earlier due to excessive tangling of the flagella.

μ	AIPTS	Total Iterations	Sim End [sim s]
0.1	3.01	6.02×10^5	250
0.2	3.01	6.04×10^5	250
0.3	3.61	7.25×10^5	250
0.4	4.89	9.83×10^5	250
0.5	6.67	1.34×10^6	250
0.6	8.71	1.76×10^6	250
0.7	14.47	2.72×10^6	235.89
0.8	14.16	1.89×10^6	180.98
0.9	11.1	1.05×10^6	142.72
1.0	11.65	1.02×10^6	135.32

As μ increases past 0.7, the tangling happens earlier and earlier as shown. Furthermore, we observe that the number of average iterations starts to increase as μ increases. This is in line with our expectations as larger μ values result in greater sticking.

5. Conclusion

In this paper, we introduced an improved version of our fully-implicit and penalty-based frictional contact method, Implicit Contact Model. To test the performance of our contact model, we formulated an end-to-end simulation framework for the novel and difficult contact scenario of flagella bundling in viscous fluid. For this contact problem, we showed that IMC has comparable

performance to the state-of-the-art while maintaining faster convergence. Furthermore, we showcased visually convincing frictional results in an imaginary viscous environment where friction is non-negligible.

For future work, we wish to improve upon the stability and robustness of our friction model. Despite the implicit formulation, the number of iterations necessary to converge starts to increase as μ increases. Another interesting avenue of research is the use of deep learning to learn physics-based dynamics for simulation. Neural networks, when properly trained, have been known to be able to generate nearly identical outputs as numerical simulations while achieving orders of magnitude reduction in computation. Thus, utilizing the computational efficiency and differentiability of neural networks while maintaining physical realism is a promising direction.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at <https://doi.org/10.1016/j.eml.2022.101924>.

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