Zipping and entanglement in flagellar bundle of E. coli: Role of motile cell body

Tapan Chandra Adhyapak* and Holger Stark†

Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany
(Received 29 March 2015; revised manuscript received 20 August 2015; published 2 November 2015)

The course of a peritrichous bacterium, such as E. coli, crucially depends on the level of synchronization and self-organization of several rotating flagella. However, the rotation of each flagellum generates countermovements of the body which in turn affect the flagellar dynamics. Using a detailed numerical model of an E. coli, we demonstrate that flagellar entanglement, besides fluid flow relative to the moving body, dramatically changes the dynamics of flagella from that compared to anchored flagella. In particular, bundle formation occurs through a zipping motion in a remarkably rapid time, affected little by initial flagellar orientation. A simplified analytical model supports our observations. Finally, we illustrate how entanglement, hydrodynamic interactions, and body movement contribute to zipping and bundling.

DOI: 10.1103/PhysRevE.92.052701

PACS number(s): 87.16.Qp, 47.63.Gd, 87.10.Pq, 87.17.Jj

I. INTRODUCTION

Understanding the self-propulsion of microorganisms poses utmost challenges involving rich and complex physics [1–7]. Bacteria are among the simplest and widely studied of such systems [8–13]. Yet, only recently have we been able to explore in full detail the underlying physics involved [14–26]; much of this, however, is still to be apprehended. Propulsion of peritrichous bacteria, such as E. coli, is generated by the rotation of a bundle of several helical propellers, called flagella. Flagella are passive filaments rotated at one end by rotary motors embedded in the cell wall [27]. The level of synchronization and self-organization of rotating flagella crucially decides the swimming course of the cell body to which they are attached making it either propel or tumble. However, the dependency is not one sided: The rotary motors that rotate each flagellum also produce systematic body movements, which in turn affect the flagellar dynamics. Whereas the rotating cell body drags the proximal ends of flagella with it, the distal ends cannot keep up due to friction with the surrounding fluid. In understanding flagellar synchronization and bundling dynamics, focus has so far been given primarily on hydrodynamic interactions and elastic properties of flagella [19,21,25,26,28,29]. Although, body movement is speculated to play an important role too [9,30], knowledge of its detailed impact is still lacking.

The cell body moves in response to the forces and torques acting on it [31]. It translates due to the thrust force generated by the rotating bundle of flagella in the surrounding fluid medium at a low Reynolds number. It also has to rotate since the torque on the body has to balance all motor torques acting by the rotating bundle of flagella in the surrounding fluid [19,21,25,26,28,29].

II. GOVERNING EQUATIONS AND NUMERICAL METHODS

A. Dynamics of the flagella

We first summarize our approach to describe the dynamics of the cell body with multiple flagella in an unbounded fluid of viscosity η. We treat each flagellum as a slender body with centerline r(s) parametrized by the arc length s. By affixing the orthonormal tripod \{e₁(s), e₂(s), e₃(s)\} at each point on the centerline, where e₃ is the local tangent and e₁ and e₂ are unit vectors along the principal axes of the flagellar cross section, one can fully characterize the bent and twisted flagellum. Dynamics of the flagellum now is governed by Langevin equations for r(s) and the twist angle φ(s) about the centerline [17].

\[
\begin{align*}
\frac{\partial}{\partial t} r &= \mu_r (F_{el} + F_s + F_{th}) + v_h, \\
\frac{\partial}{\partial s} \phi &= \mu_c (T_{el} + T_{th}).
\end{align*}
\]
Here, we separate the velocity contribution $v_0$ due to hydrodynamic interactions from local terms and denote local forces and torques by $F$’s and $T$’s, respectively. Self-mobilities $\mu_i = e_i \otimes e_i / \gamma_i + (1 - e_i \otimes e_i) / \gamma_i$ and $\mu_\perp = 1 / \gamma_\perp$ are expressed in terms of friction coefficients per unit length. For the flagellum of an E. coli they are $\gamma_i = 1.6 \times 10^{-3} \text{pN s} \mu m^{-2}$, $\gamma_\perp = 2.8 \times 10^{-3} \text{pN s} \mu m^{-2}$, and $\gamma_\perp = 1.26 \times 10^{-6} \text{pN s}$ [20]. Thermal forces $F_{th}$ and torques $T_{th}$ are shown for completeness. Although these are predicted to play an important role during rotation-induced polymorphic transformations of a flagellum [20], they are negligible in our present study [21] and are ignored.

Elastic forces and torques $F_{el} = -\delta F / \delta r$ and $T_{el} = -\delta T / \delta \varphi$, respectively, are derived from the total elastic free energy $F[r(s), \phi(s)]$ of the flagellum, the form of which is obtained as follows. The rotational strain vector $\Omega$ moves the material tripod along the flagellum: $\delta \varphi = \Omega \times e_i$; $i = 1, 3$. Therefore, its components completely characterize the instantaneous flagellar configuration [20]. A small deformation $\delta \Omega = \Omega - \Omega^0$ from the normal helical ground state $\Omega^0 = \{0.0, 1.3, -2.1\}$ (in $1/\mu m$) [17,32] needs the Kirchhoff elastic free energy density [33], $f_3(\Omega) = (A/2)\{d(\Omega_1)^2 + (d\Omega_2)^2 + (C/2)(d\Omega_3)^2\}$. For E. coli, we choose an isotropic bending rigidity $A = 3.5 \text{pN mm}^2$ (assuming a circular flagellar cross section) and the twist rigidity $C = 0.09$. Integrating over the length of the flagellum, we obtain $\mathcal{F}[r(s), \phi(s)] = \int ds f_3(f_1 + f_3)$ when we include a stretching free energy density $f_8 = K(\delta r)^2/2$ with $K = 10^3 \text{pN}^2$ [17].

### B. Steric and hydrodynamic interactions

To proceed, we discretize Eqs. (1) and (2) by considering discrete positions $\mathbf{r}_i \equiv r_i(\lambda_i)$ along each flagellum and by assigning $[e_1(i), e_2(i), e_3(i)]$ to the straight segment of length $h$ between $\mathbf{r}_{i-1}$ and $\mathbf{r}_i$ (see Fig. 1). Excluded-volume interactions among flagella are enforced by the steric force $\mathbf{F}_s(\mathbf{r}_i) = \sum_j \mathbf{F}^s(h - h_j)/h$. Here, the summation runs over all overlaps occurring within $[r_{i-1}, r_{i+1}]$ of a given flagellum, and $\mathbf{F}^s$ is the steric force at a distance $h_j$ from $\mathbf{r}_i$, appropriately decomposed to act on the discrete points (details of the implementation are given in Appendix A). $\mathbf{F}^I$ derives from the Lennard-Jones potential $U_{IJ}(r_{ij}) = (\sigma / 6)(\sigma / r_{ij})^2 - (\sigma / r_{ij}^6)\theta(2^{1/6}\sigma - r_{ij})$. We truncate it at the minimum using the heaviside step function $\Theta(x)$, where $r_{ij}$ is the minimal distance between the centerlines of the two approaching flagella and $F_0$ is the strength of the steric force at $r_{ij} = \sigma$. We choose $F_0 = 0.8 \text{pN}$ and adjust $\sigma = 4a$ with $a$ as the cross-sectional radius of the flagellar filament, ensuring numerical stability during entanglement in all situations.

Finally, to include hydrodynamic interactions between the flagella, we treat each discrete point $\mathbf{r}_i$ as a sphere of radius $a$ and set $\mathbf{v}_b(\mathbf{r}_i) = \sum_j \mu_{ij}(\mathbf{r}_i) \mathbf{F}(\mathbf{r}_j)$. Here, $\mu_{ij}$ is the Rotne-Prager mobility matrix [34] for spheres at $\mathbf{r}_i$ and $\mathbf{r}_j$, $\mathbf{F}(\mathbf{r}_j)$ is the local force at $\mathbf{r}_j$, and the summation runs over all points of both flagella. We neglect subleading effects from hydrodynamic interactions due to rotation of the spheres. Furthermore, neglecting hydrodynamic lubrication for close flagella is justified for thin filaments and the presence of asperities in real flagella [35] (details of the argumentation are given in Appendix B).

### C. The cell body, flagellar hook, and rotary motor

We model the cell body by a spherocylinder of length $L_b = 2.5 \mu m$ and width $d_b = 0.8 \mu m$ [27] (see Fig. 1). Point $r_0$ of each flagellum is fixed on the body surface, and a motor torque $T_m = T_m \mathbf{m}$ drives the flagellum by rotating the motor tripod $\{e_0(0), e_0(0), e_0(0) = \mathbf{m}\}$ at $r_0$. This tripod couples to the main part of the flagellum through the Kirchhoff elastic free energy density $f_k$ where we set $A \to 0$ and $C \to 3C$ (any nonzero but small bending rigidity of the hook does not significantly affect our results as shown in Appendix C). Thus, the driving torque is transferred to the flagellum through a hook that acts as a universal joint with low bending and high twist rigidities [36] allowing the first flagellar segment along $e_3(1)$ to be at any angle to $\mathbf{m}$. In response, the body moves and rotates with velocities $\mathbf{v}_b = \mu_b^s \mathbf{F}_b$ and $\mathbf{w}_b = \mu_b^T(T_b + T_m)$, respectively. Here, $\mathbf{F}_b$ and $T_b$ are the respective force and torque (relative to the body center) resulting from the forces $\mathbf{F}_{el} + \mathbf{F}_s$ that act on the flagellar anchoring points. For the mobilities $\mu_b^s$ and $\mu_b$, we use the analytically available values for a prolate spheroid of aspect ratio $L_b/d_b$ [37]. The angle $\phi_m$ between $\mathbf{m}$ and $e_{34}$ is expected to differ from 90° because of, for example, a locally curved body surface. We adjust $\phi_m = 55°$ to obtain a ratio for the bundle-to-body rotation within the experimentally observed range [9]. Furthermore, we employ the same potential $U_{IJ}(r_{ij})$ to describe the excluded-volume interaction between the body and the flagella, where $r_{ij}$ now is the minimal distance between the body surface and any $\mathbf{r}_i$ on a flagellum.

### III. RESULTS

Figure 2 shows typical snapshots of the bacterium moving towards the left with the flagella in their normal left-handed helical form. The snapshots were obtained at regular intervals from a particular simulation run. Quantitative details of the corresponding flagellar dynamics are presented in Fig. 3. At time $t = 0$ ms, flagella start with an angle $\Phi$ between their axes. As time progresses, they rotate counterclockwise about their axes (as viewed from behind the cell) when driven by a positive motor torque $T_m = 3.4 \text{pN} \mu m$ [9,17]. Simultaneously, the cell body performs a counterbalancing clockwise rotation and translates because of the thrust force generated by the flagella. The resultant flagellar evolution
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is complex. It involves entanglement and large bending of flagellar axes. We now present a detailed investigation of the flagellar dynamics.

A. Synchronization of flagellar rotation

To quantify synchronization of flagellar rotation in such situations, we need to compare the respective tripod vectors \(\mathbf{e}_i(i)\) and \(\tilde{\mathbf{e}}_i(i)\) from the two flagella at the same flagellar position \(i\). Therefore, we introduce the effective phase difference \(\theta(i) = \cos^{-1}[\mathbf{e}_i(i) \cdot \tilde{\mathbf{e}}_i(i)]/\pi\) with \(\tilde{\mathbf{e}}_i(i) = \mathcal{R}[\mathbf{e}_i(i)]\), where \(\mathcal{R}\) rotates the tangent vectors onto each other \([\tilde{\mathbf{e}}_i(i) = e_i(i)]\) about the axis \(\mathbf{e}_3(i) \times \tilde{\mathbf{e}}_3(i)\). Starting from a nonzero initial value, the contour average \(\langle \theta \rangle\) quickly drops towards zero, and the flagella reach a nearly synchronized rotational state after about 10 ms [see Fig. 3(a)]. This is also reflected in the snapshot at 10 ms shown in Fig. 2 where the phases of both flagella clearly match. The initial regime remains unaffected when changing the initial value of \(\langle \theta \rangle\). It is completely determined by hydrodynamics since steric forces are zero as documented by the inset of Fig. 3(a). The subsequent, almost linear decrease in \(\langle \theta \rangle\) towards full synchronization coincides with bundle formation, which we discuss now.

B. Enhanced bundle formation through zipping: role of flagellar entanglement

Although cell-body movements only quantitatively change synchronization dynamics, they dramatically influence bundling dynamics compared to the case of anchored flagella [18,19,21]. At \(t \approx 10\) ms proximal portions of the flagella start to wrap around the body axis [see Fig. 2] after synchronization has already proceeded considerably. This marks the beginning of bundling near the cell body, whereas the rest of the flagella are still apart. With time the front of the bundled portion advances away from the body, gradually drawing remaining loose flagellar portions into the bundle. The growth of the bundled portion thus resembles a zipping motion where the zip starts at a point near the body and continues until the whole of the flagella have joined the bundle.

To quantify these findings, we define the bundled portion as the part of a flagellum for which all its points are at distances \(<2R\) from the other flagellum. We choose \(R = 0.22\) \(\mu m\) to be the equilibrium radius of the helical flagellum. The bundle length \(l_l\) is then measured from the cell body to the bundle front normalized by the axial length \(L_{w}\) of a flagellum. As seen from Fig. 3(b), zipping takes place within approximately 5–20 ms. During this period, after an initial sharp increase \(l_l\) grows almost linearly with time. Furthermore, for the studied range of opening angles \(\Phi\) the bundling time only varies by about 10 ms. Therefore, it is always much smaller than the total tumble time of 150–450 ms [8]. So, bundling during a tumble event is remarkably independent of the extent to which a flagellum is thrown out of a bundle. This gives crucial insight into the locomotion of a bacterium since bundling without supporting body movements takes much longer.

Flagellar entanglement is observed to play an important role in all the findings mentioned above. During zipping, the steric force density \(f_c = |\mathbf{F}_x|/L\), where \(L\) is the length of a flagellum, is found to build up until bundling completes after which \(f_c\) declines rapidly [inset, Fig. 3(b)]. Due to viscous drag and flagellar flexibility, parts of the flagella not in the bundle hardly follow the cell-body rotation (see movie M1 in the Supplemental Material [38]). As a result, proximal portions of the flagella not only start to wrap around the body axis, but also get entangled [snapshot at \(t = 10\) ms, Fig. 2]. This drastically enhances flagellar bundling: Further rotation of proximal ends is possible only when the entangled front proceeds away from the body, gradually bringing the rest of the flagella quickly into the bundle. A simplified analytical model discussed below further supports these observations. A correlation between \(f_c\) and the slow linear decline of \(\langle \theta \rangle\) mentioned earlier is clear from the inset of Fig. 3(a). Although flagella in the bundle
are synchronized, the local phase differences \( \theta(i) \) of their free ends fluctuate strongly until entanglement forces them into the bundle. This is observed to be responsible for the delayed slow decline of \( \langle \theta \rangle \).

C. Simplified analytical treatment capturing zipping in bundle formation

A simplified model for the zipping dynamics takes into account flagellar entanglement at the bundle front and fluid flow in the body-fixed reference frame. The latter occurs with respective translational and rotational velocities \( v_c = -v_b \) and \( \omega_c = -\omega_b \) [see Fig. 3(c)]. Accordingly, the length of the bundle grows with speed \( dl/dt \), and the angle \( \psi = 90^\circ - \Phi/2 \) varies in time according to

\[
\frac{dl}{dt} = v_c + \frac{\omega_c R}{\cos \psi} \quad \text{and} \quad \frac{d\psi}{dt} = \frac{v_c \cos \psi}{L_{ax} - l_f}.
\]

Like in a zipper the free portions of the rotating flagella are dragged into the bundle front \( P \) with the helical phase velocity \( v_c \). They are perfectly fit into the bundle; hence \( l_f \) grows with the same speed \( v_c = \lambda_f v_f \), where \( \lambda_f \) is the helical pitch and \( v_f \) is the frequency of rotation. Second, the surrounding fluid wraps the free flagellar portions with an angular velocity \( \omega_c \) onto the bundle cylinder. So, flagella are dragged with an additional speed \( \omega_c R/\cos \psi \) into the bundle front, where \( R \) is an effective bundle radius. Finally, the translational flow rotates the flagellar tip with speed \( v_c \cos \psi \) about the bundle front \( P \), which gives the angular velocity \( d\psi/dt \). Equations (3) are solved for \( l_f(t) \) using parameter values measured from our simulations with \( R \) and \( l_f(t = 0) \) adjusted for the best fit. The results plotted as dashed lines in Fig. 3(b) agree well with our simulation results, strengthening the interpretation of our observations discussed above.

IV. COMPARISON OF EFFECTS OF BODY MOVEMENT AND STERIC AND HYDRODYNAMIC INTERACTIONS

To obtain further insight into flagellar dynamics, we perform a comparative study to judge the relevance of cell-body movements and various flagellar interactions. The results are presented in Fig. 4. We consider the standard simulation run performed at \( \Phi = 23^\circ \). Its results [curves (i) in Fig. 4] are compared with those obtained from new simulations where either body movements or flagellar interactions are ignored. The impact of body rotation on the synchronization dynamics is more pronounced than that of body translation [inset, curves (iii) and (iv)]. Without body rotation, \( \langle \theta \rangle \) converges more slowly towards zero, qualitatively resembling the results of anchored flagella [26]. However, absence of body translation does not affect the outcome much. Hydrodynamic interactions (HIs) between flagella are important in reproducing the standard result of the full simulation [inset, curves (i) and (ii)]. However, we find that synchronization is even possible without HI contrasting the situation of anchored flagella where HIs between flagella are known to be essential [26]. Interestingly, cell-body movement is sufficient to synchronize flagella, similar to findings for Chlamydomonas in Ref. [39].

Bundling dynamics is affected with a similar trend. Although bundling is delayed by approximately 10 ms in the absence of HIs between flagella, the absence of body translation is less severe [curves (i), (ii), and (iv) in Fig. 4]. There is no bundle formation in the absence of axial body rotation [horizontal line as curve (iii)] because the body reorients and slows down translation, resulting in an unusual buckling of flagella away from each other. More significantly, when we follow Ref. [30] and allow temporal evolution of each flagellum affected only by body movement but not by either HI or steric interactions, bundling gets significantly delayed by about 30 ms [curves (v) and (vi)].

V. CONCLUSION

To conclude, we present a detailed modeling of an E. coli with two flagella and a motile cell body. This allows us to probe bacterial propulsion on a yet experimentally inaccessible level. The complex role of flagellar polymorphism is ignored for simplicity. In principle, it can be probed extending our model [17]. We demonstrate that compared to the situation of anchored flagella, flagellar dynamics close to real conditions is strikingly altered by body movements. Times to bundle and synchronize are dramatically reduced. In particular, flagellar entanglement helps bundling to proceed quickly like a zipping motion, which we rationalize in a simplified model. Furthermore, we demonstrate that body movement and flagellar entanglement lead to rapid bundling and synchronization even when hydrodynamic interactions are neglected. Our findings are important in explaining experimentally observed times scales as mentioned above.

Real E. coli possess between four and eight flagella, which are randomly distributed around the cell surface. Consideration of such a situation does not alter our results qualitatively [40]. Furthermore, our model is robust under reversal of flagellar rotation back and forth. Thus it can already simulate bacterial tumbling although without polymorphism [38].

Finally, more and more artificial microswimmers using different swimming mechanisms have been and are constructed [41]. We provide here an example how one develops a model for exploring and ultimately understanding the biomechanics of microswimmers.
ACKNOWLEDGMENTS

We are grateful to R. Vogel for useful discussions and providing key insights to the numerics involved. We also acknowledge D. Alizadehrad, G. Gompper, P. Kanelh, O. Pohl, C. Prohm, R. Winkler, and A. Zöttl for helpful discussions. We thank the VolkswagenStiftung for financial support within the program “Computational Soft Matter and Biophysics” (Grant No. 86 801).

APPENDIX A: STERIC FORCE BETWEEN FLAGELLA

In this section we elaborate on our numerical scheme to calculate the steric forces \( \mathbf{F}_s(r_i) \) with which one flagellum acts on the point \( r_i \) of the other flagellum. We consider two flagellar segments along the respective tangent vectors \( \hat{t} \equiv \mathbf{e}_i(i + 1) \) and \( \hat{t}' \equiv \mathbf{e}'_i(k + 1) \) as illustrated in Fig. 5(a). The segments belong to the two flagella described by the centerlines \{\( r_i \)\} and \{\( r'_i \)\}, respectively.

Determining the interaction of two segments from different flagella can be divided into two cases. First we check if one end of a segment approaches the other segment closer than the cutoff distance \( 2/\kappa \sigma \) of our steric potential \( U_{\text{LJ}} \) [see Figs. 5(b) and 5(c)]. The separation vector \( \mathbf{G} \) points from the end of the approaching segment to the other segment and is normal to the latter. If this case does not produce an interaction, we consider the second case illustrated in Fig. 5(a). Here, the inner parts of the two segments interact along the direction with the shortest distance. So, we have [42]

\[
\mathbf{G} = r_i + h_j \hat{t} - r'_j - h'_j \hat{t}',
\]

(A1)

with

\[
h_j = \frac{\left| (r_i - r'_j) \cdot \hat{t} \right| \hat{t}}{1 - (\hat{t} \cdot \hat{t})^2},
\]

(A2)

\[
h'_j = \frac{\left| (r'_j - r_i) \cdot \hat{t} \right| \hat{t}}{1 - (\hat{t} \cdot \hat{t})^2},
\]

(A3)

where \( h_j \) and \( h'_j \) are the respective distances from \( r_i \) and \( r'_j \) to the corresponding proximate points \( D \) and \( E \).

The steric force \( \mathbf{F}^i_j \) acting at \( D \) on the flagellum \{\( r_i \)\} is now readily obtained from the truncated Lennard-Jones potential \( U_{\text{LJ}} \) defined in the main article as

\[
\mathbf{F}^i_j = -\frac{d}{d \mathbf{G}} U_{\text{LJ}}(\mathbf{G}).
\]

(A4)

We now replace \( \mathbf{F}^i_j \) by an equivalent system of forces \( \mathbf{F}^i_{i+1} \) and \( \mathbf{F}^i_{i+1} \) that act on the discrete points \( r_i \) and \( r_{i+1} \), respectively, and are both parallel to \( \mathbf{F}^i_j \). The effect of \( \mathbf{F}^i_j \) on the flagellar segment along \( \hat{t} \) is same as the combined effect of the forces \( \mathbf{F}^i_i \) and \( \mathbf{F}^i_{i+1} \) if both the original and the new system of forces produce the same resultant force and torque on the center of mass \( C \) of the segment,

\[
\mathbf{F}^i_s = \mathbf{F}^i_i + \mathbf{F}^i_{i+1},
\]

(A5)

\[
\left( \frac{h_j}{2} - h_j \right) \mathbf{F}^s_j = \frac{h_j}{2} \left( \mathbf{F}^i_j - \mathbf{F}^i_{i+1} \right).
\]

(A6)

This implies \( \mathbf{F}^i_j = \mathbf{F}^i_i (h_j - h_j)/h \). Thus, summing over contributions coming from all overlaps occurring within \{\( r_{i-1}, r_{i+1} \)\}, we finally obtain the total steric force at \( r_i \) as

\[
\mathbf{F}_s(r_i) = \sum_j \mathbf{F}^i_j = \sum_j \mathbf{F}^i_j (h_j - h_j)/h.
\]

APPENDIX B: EFFECT OF HYDRODYNAMIC LUBRICATION FORCES

In this section we follow the argument in Ref. [35] to show that near field hydrodynamic lubrication forces on slender flagella are not strong enough to prevent actual physical contact. For simplicity we consider two straight flagella with their axes of symmetry perpendicular to each other [Fig. 5(a)]. A general configuration does not affect our argument much. The lubrication force resisting the normal approach of the flagella towards each other is given by [35]

\[
F_{\text{hub}} = -\frac{6\pi \eta a^2}{G} \frac{dG}{dt},
\]

(B1)

where \( G(t) \) is the separation at time \( t \) and \( a \) is the radius of the flagellar filament. Then, a change in gap thickness, under the action of a force \( F_f \) normal to one of the flagella, is obtained by solving the condition of force balance \( F_f = F_{\text{hub}} \), yielding

\[
G(t) = G(0) \exp \left( -\frac{F_f}{6\pi \eta a^2} t \right).
\]

(B2)

FIG. 5. (Color online) Numerical scheme to determine the steric force acting at the discrete point \( r_i \) of a flagellum. The vector \( \mathbf{G} \) of minimal approach between two interacting segments is determined by separately treating the situation when the segments approach each other away from their end points (a) from the one where the minimal approach occurs at one of the ends [(b) and (c)]. Orientations of \( \mathbf{G} \) and the local steric force \( \mathbf{F}^i_j \) relative to the segments are depicted.

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where \( G(0) \) is a finite distance above which lubrication is negligible. We estimate the normal force as \( F_f \sim L \gamma_\perp v_f \), where \( \gamma_\perp = 2.8 \eta \) is the transverse friction coefficient per unit length of a flagellum of total length \( L \) and \( v_f \) is a typical transverse velocity. Typically \( v_f \sim \omega_f R \) with \( \omega_f \) as the frequency with which a helical filament of radius \( R \) is rotated about its axis. So, after a time on the order of \( T_c = \frac{2 \pi}{\omega_c} \), where \( \omega_c \) is the body rotation rate and taking \( \omega_f/\omega_c \sim 10 \), we have

\[
G(\sim T_c) \propto G(0) \exp \left( -10 \frac{LR}{a^2} \right) \approx 0
\]

for values of \( L, R, \) and \( a \) used in the main paper. Hence, for typical values of driving forces and on the relevant time scale of bundling, lubrication forces cannot prevent the filaments from approaching each other very closely. The separation would be smaller than asperities present in their surfaces. This means lubrication is negligible for flagellar bundle formation. Filaments do come into physical contact experiencing the steric forces described in the previous section.

**APPENDIX C: EFFECT OF NONZERO BENDING RIGIDITY OF THE HOOK**

Figure 6 shows that for values of \( A_h \) as high as 0.02 \( \text{pN} \mu\text{m}^2 \), there is no significant change in the zipping and synchronization dynamics. Time to complete the bundle changes only slightly, and the slope of the curve for the growth of bundle length remains unaffected [Fig. 6(a)]. Similarly, the drop in phase difference follows the same trend [Fig. 6(b)].

The only known experimental value of the bending rigidity of the hook of an \( E. coli \) flagellum is \( A_h = 1.0 \times 10^{-5} \text{pN} \mu\text{m}^2 \) [43]. In comparison to the nonzero values studied in Fig. 6, such a small bending stiffness does not at all affect the synchronization and zipping dynamics presented for zero bending rigidity in the main text.

**APPENDIX D: SENSITIVITY TO DIFFERENT PARAMETERS**

As evident from Fig. 7(a), our observations are robust against changes in the values of the strength of steric interactions \( F_0 \). Also, changes in the flagellar bending rigidity \( A \) do not affect zipping and entanglement dynamics [Fig. 7(b)]. Other parameters are either set to experimental values or are found not to affect our predictions.

**APPENDIX E: MOVIES SHOWING ZIPPING AND SYNCHRONIZATION**

See Supplemental Material Ref. [38].

(1) \( M1.avi \): Two flagella with symmetric attachments and \( \Phi = 90^\circ \).

(2) \( M2.avi \): Four flagella with nonuniform attachments: Bundle aligned to body axis.

(3) \( M3.avi \): Four flagella with nonuniform attachments: Bundle inclined to body axis.

*Color scheme.* Different colors of flagella in all the above movies are just for visual clarity of individual flagella in a bundle.
See Supplemental Material Ref. [38].

1) M4.avi. Two flagella with symmetric attachments and \( T_m = \pm 3.4 \) pN m.

Color scheme. The blue color indicates a counterclockwise rotated (\( T_m > 0 \)) flagellum, and the red color indicates a clockwise rotated (\( T_m < 0 \)) flagellum.

[38] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevE.92.052701 for movies M1, M2, and M3 showing synchronization and bundling of two and four flagella and the movie M4 showing a tumbling event upon reversal of flagellar rotation. Detailed lists of the movies are given in Appendices E and F, respectively.
[40] Simulations performed with four flagella, emanating from nonuniform locations on the cell body and resulting in a bundle either parallel to or inclined at an angle with the body axis, show the same qualitative bundling and entanglement dynamics as discussed in the main text (see movies M2, M3, and the Supplemental Material [38]).