Geometry of Axoneme-like Filament Bundles

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Abstract

We develop a formalism that describes the bending and twisting of axoneme-like filament bundles. We obtain general formulas to determine the relative sliding between any arbitrary filaments in a bundle subjected to unconstrained deformations. Particular examples for bending, twisting, helical and toroidal shapes, and combinations of these are discussed. Resulting equations for sliding and transversal shifting, expressed in terms of the curvature and torsion of the bundle, are applied to flagellar bend data. We prove that simultaneous combination of twisting and bending can produce a drastically drop in the sliding, by decreasing bending rigidity.

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1 Introduction

Internally generated oscillations of bending and twisting filaments are of particular interest for the study of cellular biomechanics and motility in flagellated cells. Flagella and cilia control the motility of single cell organisms and fluid flow in multicellular tissues [1]. A current gap in the modeling of flagellar motion is a mathematical description of the influence of a local deformation on the global shape (and dynamics) of the filament bundle. Several groups have addressed deformations [2-14], whereas [15, 16] have examined the effects of imposed bends on the global curvature sperm flagella. However, as yet, a means to calculate the precise effects of a local bend/twist/slide among the individual filaments of the axoneme on the global geometry of the flagellum has not been presented. In the present paper, we begin to address that gap by developing a mathematical formalism based on the differential geometry of curves, on the theory of motion of curves, and on functional approaches in order to obtain a new and general formula for calculating the relative sliding between any two arbitrary filaments in a bundle of filaments subjected to a 3-d deformation.

To gain a better understanding of how flagellar bends influence flagellar geometry, we analyze the deformations of axoneme-like filament bundles [1,2-4,7-15]. Microscopic dynamical models that describe the occurrence of regular beats, and waves in cilia and flagella are based on internally driven motion controlled by molecular motors [2-6,8,10,14,15,17-25]. In these models the flagellum or axoneme is described as a quasi-continuum quasi-flexible cylindrical filament bundle containing the distribution of molecular motors. In the presence of ATP, the motors generate relative local forces, and local torques, and the resulting internal stress induces a relative sliding motion of the filaments, which ultimately leads to the propagation of bending waves [3,5,17,26]. There is also experimental evidence of the direct influence of geometrical properties of the filament bundle upon the dynamics. There are experiments that show how locally induced sliding produces global bending, in order to conserve the total curvature of the bundle [16]. Another important motivation for the mathematical study of the geometry of filament bundles is the intrinsic regulation of molecular motors through geometry changes induced by bending [17].

Theoretical models approaching bundle deformations and sliding are also used to explain symmetry breaking in the nonlinear dynamics of stiff polymers [28], coupling between internal forces and relative sliding [5], or analysis of helical structures for modeling bending and twisting of bacterial flagella, etc.

In this article we introduce the bundle of filaments model and its deformation, and we obtain in Section 2 a sliding expression for bending, in the case of parallel and non-parallel filaments. In Section 3 we introduce the twisting of the bundle and its influence on the sliding equation. We provide expressions for cylindrical helix in Section 3.1, and also for arbitrary helices, and present numerical calculation for a helix winding around another helix in section 3.2. Examples of sliding distribution in planar waves, rigid rotation and helical motion are also discussed. In Section 4 we couple bending and twisting for parallel
filaments, and in Section 5 we study the most general situation of the sliding produced by bending/twisting in arbitrary shapes and non-parallel filaments. The general equation is verified by reducing it to the known 2-d cases in Section 5.2.

The results in this article describe a mathematical formalism for predicting the precise position of any filament within a deformed bundle, which can be used both in numerical or analytical modeling. This formalism is also useful in experimental studies to predict local or global distributions of forces and torques (activity of molecular motors, for example) derived from experimentally observed shapes. This formalism can be used to better understand the dynamics of a flagellum, the structure of bends and waves, the importance of boundary conditions on flagellar shape dynamics, and cellular propulsion systems that depend on flagella like hair-like systems.

2 Bending deformations

The axoneme consists of a tubular structure of 9 pairs (doublets) of filaments (microtubules), and in most, but not all organisms, the axoneme contains one central pair of filaments which is connected to the other doublets by protein spokes [1-3,17,26]. The molecular motors form arms between the outer doublet microtubules, resulting in a local relative sliding displacement between adjacent microtubules [2,5,17]. In addition to a relatively parallel shifting along the longitudinal axis of the axoneme (providing microtubules are free to move), the boundary conditions imposed on the doublets creates bending in different directions and twists around the lateral axis of symmetry. Bending is the result of holding the doublets together during a shift (quasi-elastic constrains) produced by the local distribution of axial forces and normal torques along the flagellum. Local twist results if all the active pairs slide in the same direction due to torque oriented along the local flagellum axis, which also generates longitudinal compression/extension.

Local sliding and twist does not simply correspond with the local action of motors, since active bending in one region can induce bending in some passive sections of the bundle. For example, if the longitudinal displacement of the filaments is restricted at both ends of flagellum, the total sliding integrated along the flagellum should be zero. So due to the mechanical constrain of the total system, regions with positive bending (considered by convention as positive) should be compensated with regions of negative bending, even if those regions are not motor active. Very recent experiments performed with micron calibrated glass needles show if a bend is forced into an inactive flagellum, the other half bends in opposite direction trying to keep the total integral curvature zero [15].

In the present model, we study the 3-dimensional deformations of an axoneme-like structure consisting of a bundle of filaments. We define a bundle of filaments $\mathcal{B}$ as a family $\bar{r}_k(\alpha) : [0, \alpha_{\text{max}}] \to \mathbb{R}^3$ of $N$ parameterized regular curves ($k = 1, 2, \ldots, N$) where $\alpha$ is an arbitrary parameter, common to each curve associated to each filament. Between
any two filaments $k$ and $j$ we can write

$$
\vec{r}_k(\alpha) = \vec{r}_j(\alpha) + d_{kj}(\alpha)\vec{n}_j(\alpha) + e_{kj}(\alpha)\vec{b}_j(\alpha).
$$  

(1)

The unit vectors $\vec{n}_j(\alpha)$ and $\vec{b}_j(\alpha)$ are the normal and the binormal directions to filament $j$ at $\alpha$ [29,30]. The functions $d_{kj}, e_{kj}$ are the structure parameters of the bundle, and $k$ runs $k = 1, 2, \ldots, N, k \neq j$. These structure parameters determine the spatial separation measured in the principal normal plane of filament $j$, between the reference filament $j$, and any other filament $k$ in the bundle. If these parameters are constant versus $\alpha$ for all $j, k = 1, \ldots, N$, we refer to this bundle as parallel: each two filaments are separated by constant transversal distances.

We define the relative sliding of filament $j$ with respect to filament $k$, at a point $\vec{r}_k(\alpha)$ on filament $k$ by the expression

$$
\delta_{jk} = [\vec{r}_j(\alpha^*(\alpha)) - \vec{r}_k(\alpha)] \cdot \vec{t}_k(\alpha),
$$

where $\alpha^*(\alpha) : [0, \alpha_{max}] \rightarrow [0, \alpha_{max}]$ is the inverse image $\alpha^* = (\vec{r}_j)^{-1}$ of the point of intersection between filament $j$ and the normal plane to the filament $k$ at $\alpha$, chosen such that the distance between this intersection point $\vec{r}_j(\alpha^*)$ and $\vec{r}_k(\alpha)$ is minimum

$$
\vec{r}_j(\alpha^*) = \vec{r}_k(\alpha) + a_1\vec{n}_k(\alpha) + a_2\vec{b}_k(\alpha),
$$

such that $||a_1\vec{n}_k(\alpha) + a_2\vec{b}_k(\alpha)||_{(a_1,a_2) \in \mathbb{R}^2} = \text{minimum}$.

In general, the above intersection equation does not have a unique solution, because the filament $j$ can intersect the $k$ normal plane at $\alpha$ in more than one point. That is, we have more than one pair $(a_1, a_2)$ if filament $j$ bends very much and returns to this plane. However, in this article we only investigate bundles where this equation has a unique solution, at any point of every filament in the bundle. This restricts the bundles with respect to their curvature and torsion, but these are actually the interesting real situations.

Simply speaking, the relative sliding is the tangential displacement between the end points of two close enough filaments, along their (almost common) tangent. If the filaments are parallel and very close to one other, the equations describing the sliding are accurate, and we analyze such situations in Sections 2.1, 3.1 and 4. If the filaments are not parallel, and/or if they are displaced by separation distances comparable to their length, the above equations for sliding must account for a more careful geometrical analysis, which is provided Sections 2.2, 3.2 and 5.

We mention that this general definition of the sliding, i.e. $\delta_{jk}$ by using the $\alpha^*(\alpha)$ map defined as above, is a general one. In the following sections we use this definition generically, that is we express the sliding for each particular situation, in some particular convenient coordinates for that configuration. In that, in the following Eqs.(11,12,19) we use this definition in a more precise context, by the help of differential geometry of curves.

A family of more than two parallel curves are called Bertrand curves. Their curvature and torsion should be linearly dependent or any point along the filament, and the only
curve that accepts more than a Bertrand mate is the circular helix (and of course its degenerated 2-d shape, the circle) [30]. For such an ideal parallel filament bundle, where there are more than two parallel filaments, the Bertrand criterion applies, and consequently we can define only two basic types of ideal deformations: (i) **Planar bending**, where the filaments are parallel circles (degenerated helices), and (ii) **Coherent torsion**, where the filaments have helical shape. Apparently, a relative integrity of the flagellum attachments must be maintained for normal cell motility in *T. brucei* [11], but in many other real situations the connections between the pairs are neither constant nor rigid, the filaments are not parallel, and the general deformations are often intermediate variations of these two ideal types of shapes.

This situation introduces relevant considerations. On one hand, there are real situations when the shapes are close to circular bending, to cylindrical helices, or combinations of these, and the deviation from parallelism of the filaments can be treated as a rare perturbation. On the other hand, one can analytically treat the most exact general deformation by assuming that any infinitesimal deformation is a combination of circular bending and a uniform torsion, according to the Darboux theorem (an infinitesimal motion of an arbitrary smooth bundle of curves is an infinitesimal screw motion) [30]. Thus, one can integrate along the arc length, for variable radius of curvature, variable plane of bending, variable pitch (torsion) and variable radius of the helix, and obtain the precise configuration of the filaments in any shape. The most interesting experimental application of these considerations is perhaps when the flagella simultaneously bend and twist [31,32], with or without variations in the radius of the bundle [3,6,10,12,31]. None of the current mathematical formalisms for flagellar shape simultaneously accommodate all of these real-life (observed) conditions. For completeness, this approach for the geometry of filament bundles can also be applied to DNA topology [33], the intracellular cytoskeleton (both radial filaments, and conical structures) and the mitotic spindle.

### 2.1 Circular bending. Parallel filaments

In this section we describe the (ideal case) of a uniform circular 3-d bending of a bundle of parallel filaments. We consider a number of identical filaments distributed around a central filament which is plugged in the origin $O$. The un-deformed bundle, $z < 0$, is parallel to the $Oz$ axis, Fig.1.

A bending of the central filament is defined by a bending center $O_c$ placed at a distance $R_0 = |O\overrightarrow{O}_c|$ from $O$, at some angle $\phi_0$ made with the $Ox$ axis, and by the total bending angle $\alpha_{max}$ which subtends the arc $OO'$ as seen from $O_c$. The length of the bent region $OO'$ of the central filament is $L$, and we parametrize this part of the filament with the angle $0 \leq \alpha \leq \alpha_{max} = L/R_0$. Beyond the bent region, the central filament is again rectilinear, and it is confined in the vertical plane making angle $\phi_0$ with $Ox$ axis. The outer filaments (originally parallel to $Oz$ axis for $z < 0$) intersect the $z = 0$ plane in points of polar coordinates $(r\cos\phi, r\sin\phi, 0)$, namely the initial distribution of outer filaments in
the un-deformed bundle. The outer filaments bend in the same direction as the central filament, so that all filaments will uniformly bend in parallel and coaxial arcs of a circle of same length \( L \). Each filament will have a different bending radius \( R(r, \phi) = R_0 - r \cos(\phi - \phi_0) \), and its own bending center placed at \( x = R_0 \cos \phi_0 - r \sin \phi_0 \sin(\phi - \phi_0) \), \( y = R_0 \sin \phi_0 + r \cos \phi_0 \sin(\phi - \phi_0) \). From these equations we can obtain the equations of the bent filaments. To calculate the relative sliding of the filaments, we refer to the normal terminal surface of the filaments, intersecting each such curve at its end point of arc length \( L \) (the normal plane of a curve is the plane perpendicular to the tangent to the curve) [29]. For small values of \( L \) (shorter arc length, like \( \alpha_{\text{max}} < 45^\circ \)) the terminal surface of the filament bundle can be approximated (within the detectable resolution limits) as a plane. For larger \( L \) the terminal contour distorts into a complex three dimensional configuration, such as a “suction cup.”

We define the relative sliding between any two filaments as the arc length between the two corresponding terminal normal planes, measured along the filament and having the minimum radius among the two filaments \( \delta = |\alpha_{\text{max}} - \alpha'_{\text{max}}| \cdot \min\{R(r, \phi), R(r', \phi')\} \) which reads

\[
\delta = L \frac{|r \cos(\phi - \phi_0) - r' \cos(\phi' - \phi_0)|}{R_0 - \min\{r \cos(\phi - \phi_0), r' \cos(\phi' - \phi_0)\}}. 
\]

The radial sliding of a given filament (\( \delta_{\text{rad}} \)) as the arc length between its end point and its intersection with the terminal normal plane of the central filament \( \delta_{\text{rad}} = L r \cos(\phi - \phi_0)/R_0 \). The relative sliding between any two filaments placed on the circumference, tangent sliding \( \delta_{\text{tan}} \), is the difference between their radial sliding. Similarly, we calculate the tangent sliding between two parallel adjacent filaments (\( r' = r \)) separated with an angle \( \delta \phi \) along circumference

\[
\delta_{\text{tan}} = 2L \sin\left(\frac{\delta \phi}{2}\right) \frac{\sin\left(\frac{\delta \phi}{2} + \phi - \phi_0\right)}{R_0 - r \cos(\delta \phi + \phi - \phi_0)},
\]

where \( \delta ^* \phi = 0 \) if \( 0 < \Phi - \Phi_0 < \pi \) and \( \delta ^* \phi = \delta \phi \) if \( -\pi < \Phi - \Phi_0 < 0 \). Eq.(3) represents the tangent sliding between any two filaments in the bundle. To use Eq.(3), we choose one filament with angular position \( \phi \), and another one at angular separation \( \delta \phi \) from the first one (clock-wise counting). Then we apply a bending of constant radius \( R_0 \), and orientation of bending plane at \( \phi_0 \), and subtending an arc length \( L \). If we apply Eq.(3) in the range of parameters: \( r = 80nm, \delta \phi = 0.7rad, L = 12 - 20\mu m \), we obtain values for the terminal sliding in the range of \( \delta_{\text{max}} = 100 - 600nm \) which is 0.2 – 1.2% of the total length of the bundle. These numbers are in agreement with experimental measurements. They provide sliding in the same range as the sliding obtained from the frequency and velocity of sliding in [19], the protrusion of doublets measured with a very good statistics in [7].

As a verification, we notice that Eq.(3) approaches the 2-dimensional bending formula [5,20,23,26,34] in the limit \( r << R_0 \) and \( \delta \phi \to 0 \)

\[
\delta_{\text{tan}} \to 2L \frac{\delta \phi}{2} \sin\left(\frac{\delta \phi}{2} + \frac{\pi}{2}\right) \approx kr \delta \phi \, ds \to a \int k ds,
\]
where \( a = r\delta\phi \) is the linear separation between filaments, and \( k = 1/R \) is the curvature of the arc length \( L \). The radial sliding is maximum in the bending plane, while the tangent sliding has maximum values for those pairs symmetrically placed on the two sides of the bending plane.

The tangent sliding has maximum value at angles

\[
\phi_{\text{max sliding}} = \phi_0 - \frac{\delta\phi}{2} \pm \arccos \left( \frac{r}{R_0} \cos \left( \frac{\delta\phi}{2} \right) \right),
\]

which is neither in the bending plane nor orthogonal to it. For example, in the case of the \( T. brucei \) axoneme, by taking \( \delta\phi = 40^\circ \) and using Eq.(4), the maximum sliding occurs at about 76° to the right and left of the bending plane, which is very close to the separation between 3 consecutive pairs. This result agrees with the experimental evidence of the maximum change in doublet spacing occurring at doublets 3 and 8, in the geometric clutch model \([2,17]\). In a 3-d dynamical approach for curvature and twist based on the equations of momentum conservation \([3]\) this effect is explained by the action of the quasi-elastic bridges between outer doublets. From Eq.(4) we can obtain the maximum possible bend compatible with a given sliding as a function of the structural parameters of the axoneme \( r, \phi \) and \( \delta\phi \). In the case of \( T. brucei \), the maximum bend obtained is \( r/R_0 \approx 1.5 \) which gives a minimum radius of curvature of \( R_0 \approx 0.9 \mu m \) which is in good agreement with experimental measurements of curvature \([14,15,17,35]\). We can also relate the radius of bending to the maximum sliding \( \delta_{\text{tan max}} \) of the most active pair with the structural parameters. For a typical flagellum, where \( \delta_{\text{tan max}} << L \), we obtain \( R_0 \approx rL\delta\phi/\delta_{\text{tan max}} \). For a real situation we can estimate \( \delta_{\text{tan max}}/L = r\delta\phi/R = .03 \), which means that a maximum bend of \( R_0 = 5\mu m \) can be obtained if the active pairs slide with as little as 3% of their total length.

A direct application of the bending equations is shown in Fig.2, where we calculate the tangent sliding for different motions. We illustrate the density plot of the tangent sliding for each pair of filaments in a 9 pair axoneme, versus the arc length. These (diagonally) oscillating patterns in the sliding could be related with the activity of motors, showing an interesting self-organized synchronism. The patterns are in agreement with the "metachronism" recently obtained in a flagellar model \([14,36]\). In \([13]\) the authors noticed patterns similar to Fig.2 (bottom right), for small \( L \), and similar to Fig.2 (top) for short \( L \). Calculations in a similar theoretical model, approaching planar, quasi-planar and helical waveforms for the sea urchin flagellum resulted in same type of patterns \([16]\). From the numerical analysis of the relative tangent bend in different configurations in Eq.(3), we noticed that the separation of pairs \( \delta\phi \) is not very relevant to the amount of sliding. The sliding depends stronger on \( R \), but after a certain limit (\( R > 15 \div 20r \)) \( R \) is not any more relevant (asymptotic behavior).
2.2 Arbitrary bending. Non-parallel filaments

We generalize the bending deformation to more general filament bundle shapes, where all parameters can change along the arc length. Eq.(2) is valid now only at infinitesimal scale, so we substitute $L \rightarrow ds$, and integrate the slide from zero to the final length

$$\delta(L) = \int_{0}^{L} \frac{r \cos(\phi - \phi_0) - (r + \delta r) \cos(\phi + \delta \phi - \phi_0)}{R_0 - \min\{r \cos(\phi - \phi_0), (r + \delta r) \cos(\phi + \delta \phi - \phi_0)\}} ds.$$  

where $R_0, \phi_0, r, \delta r, \delta \phi$ are all functions of $s$, and min represent the minimum taken between the two expressions between $\{ \cdot \}$, for every value of $s$. The variable geometry of the filament is taken into account by the curvature $k(s) = 1/R_0(s)$ and torsion $\tau(s) = \partial \theta/\partial s$ of the filament. The position of each filament is determined by the polar coordinates $r(s), \phi_0$ and the deviation from parallelism is related to $\delta r(s), \delta \phi(s)$. This equation provides the tangent slide between a filament placed at $(r, \phi)$ angular coordinate in the bottom circumference, and another filament at coordinates $r + \delta r, \phi + \delta \phi$ (separated with $\delta \phi$ from the first one). During this bend the radius of curvature $R_0$ and the orientation of the bending plane $\phi_0$ can change, and the arc length of the bundle is $L$. All these parameters are variable versus $s$, so there is no parallel constraint, and the bend is no longer circular and uniform. However, because the twisting is not yet taken into consideration in Eq.(5), there are some restrictions on the shapes. For example, if we keep $R_1(s)$ constant, and have the bending plane rotate uniformly $\phi_0(s) \sim s$ we do not obtain a cylindrical helix, but a bend helix twisting around a toroidal shape. The full generalization of sliding and twisting, for any shape, will be discussed in Section 4.

In the following, we discuss the consequences of deviation from parallelism upon the sliding. Such deviations can be produced by tangential deviance of filaments along the circumference controlled by $\delta \phi$, or by radial deviance of filaments controlled by $r(s)$. We introduce a measurement of the tangent and the radial deviations from parallelism by

$$v_{\tan}(s) = \frac{r(\delta \phi(s) - \delta \phi(0))}{s}, \quad v_{\rad}(s) = \frac{r(s) - r(0)}{s},$$

respectively. Basically $v_{\tan} = d_{kj}$ and $v_{\rad} = e_{kj}$ from Eq.(1). The change in the sliding produce by these deviations will be measured by $\Delta \delta(s) = 1 - \delta(L, \phi)_{|\delta \phi(0), r(0), ...}/\delta(L, \phi)_{|(\delta \phi(s), r(s), ...)}$. The analytical expression of $\Delta \delta$ can be obtained from Eq.(2) through the theorem of derivation of implicit functions, but we do not go into such details. Instead, we present some numerical evaluation of the sliding for arbitrary shapes, Eq.(5), for different deviations in parallelism. In Fig.3a we illustrate the sliding of 5 parallel pairs having different positions with respect to the bending plane ($\phi = 0, \pm 30^o, \text{and } \pm 60^o$) in a cylindrical bundle. For a circular bend, for example, the sliding uniformly increases in magnitude with $L$, accordingly to Eq.(3). Then we choose different deviations from parallel and represent in Fig.3 the new sliding, for the same bend by a dotted line for each pair correspondingly (using now Eq.(5). In some of the frames we also represent the local infinitesimal slide, i.e. the integrand of Eq.(5) by the thin oscillating lines. These data clearly indicate that
minor perturbations in parallelism have only small effects on the overall sliding of the filaments.

For tangential deviation from parallelism given by an oscillatory function $\delta\phi(s) \sim \delta\phi_0 \sin(\omega s)$, with $\delta\phi_0 = 0.07\text{rad}$ taken from the clutch model in [10], there is little total change in sliding $\pm5\text{nm}$ (Fig.3 upper left frame). But, if the tangential deviation of parallelism is constantly increasing with the arc length (Fig.3b) the sliding is more enhanced. The same behavior occurs for radial non-parallelism. If the bundle radius oscillates (Fig.3c) the total new sliding follows the radius changes but the effect is still small. If we overlap the two types of deviations from parallelism, the changes in the total sliding is more significant (Fig.3d).

In this case we can have (for appropriate resonance between radial and tangent oscillations like $\delta r = \pm2 - 5\text{nm}$ and $\delta\phi(s) - \delta\phi(0) = 5^\circ$ [12]) a change in sliding of more than 200% over the total length of the bundle. In Fig.4 we show a variable radius, variable pitch bend (the shape is sketched in the left upper corner of the frame. Such situations are discussed in [12] where the authors investigate uniform (3.5$\mu$m for each doublet) and non-uniform (10$\mu$m per one doublet) tangent shift of the doublets. The thin continuous lines represent sliding of the same 5 pairs for parallel bundle. If we consider simultaneously the two types of non-parallelism, as oscillations in radius and in angular separation for each pair, we note that this ”intertwining” of filaments stabilizes and lowers the total sliding (dotted curves). The same effect is present if one considers the twisting of filament, as we will show in Section 5. Finally, in Fig.5 we present the sliding between three adjacent filaments, where the outer filaments are parallel and the middle filament-2 moves along $s$ from closer to filament-1 at one end (left cross section) to closer to filament-3 at the other end (right cross section). This case is most critical to the geometric clutch model [10,17]. We choose a simple circular bend and plotted the sliding for parallel filaments $(\delta_{12}, \delta_{23})$ (continuous curves) and the sliding for tangentially oscillating filaments (dotted curves, $(\delta_{12n}, \delta_{23n})$). Of course, by using Eqs.(2,3), we can approach more complicated distortions of the circular symmetry, like the splitting patterns observed for eukaryotic flagella and cilia axoneme [9].

3 Twisting

Long flexible structures like flagella and cilia are subject to twisting deformations in addition to bending as evidenced by both planar and helical bending patterns within the same organism under different conditions [3,6]. Internally driven bending is produced by a distribution of torques always oriented along the normal to the bundle envelope. Bending deformation may be the action of any number of pairs, while twisting deformation requires simultaneous action of two (or any even number of) pairs, since all pairs have to slide in the same direction. According to the ”geometric clutch model” [10,17] and [35], it is unlikely that the axoneme is perfectly cylindrical along its entire length, and
according to [12], the diameter of the axoneme can also oscillate. In this section, as a starting point, we calculate the filament twist in the cylindrical approximation. In the case of small changes in the bundle radius, or small radius oscillations, we can still use this cylindrical approximation, and treat the extra sliding produce by deviation from the cylindrical shapes, as perturbations. For example for a 3-d sliding model, if the twist is produced by fixed links located asymmetrically, the resulting sliding is a second-order effect, proportional to the square of the flagellum radius [2,3]. Although the approximation is reasonable, in Section 4 we unconstrain this cylindrical-parallel approximation, and we calculate the sliding produced by twisting for general shapes.

3.1 Uniform twisting. Cylindrical helix

We consider a circular bundle of radius $r$ consisting of $N$ equidistant parallel pairs of length $L$. For each pair, the two parallel filaments ($aa'$ and $bb'$) are separated by an angle $\delta\phi$, Fig.6. In a twisting deformation we assume that the upper ends $a'$ and $b'$ of the filaments are rotated with the angle $\phi$ (which is also the parameter along the filaments), while their basis remain fixed. The height of the bundle decreases from $L$ to $h$. The filaments take the shape of two parallel cylindrical helices of radii $r$, height $h$, and pitch $b$, where the pitch is defined as $h = b\phi_{max}$. By using the formula for the length of a helix $L = \sqrt{r^2 + b^2\phi}$, we obtain the twisting slide in the form

$$\delta_{\text{twist}} = \frac{ar\phi}{L} = \frac{r^2\delta\phi}{\sqrt{r^2 + b^2}},$$

(7)

where $a = r\phi$ is the linear separation between filaments in a pair. This twisting sliding is quadratic with respect to filament separation, and hence Eq.(7) is a good working approximation for situations where the deviation from parallelism are insignificant. The relative sliding for a bend is larger than the sliding for a twist for the same amount of work. That is, twisting may act like a lower gear, while bending may act like a higher gear in terms of self-propulsion. The relative shift between filaments during a twist is constant along the arc length, so shift does not increase versus length like in the case of the bending deformation.

Furthermore, twist results in compression of total length of the filament. The compression of the total length of the bundle for a given twist is $\delta L = L - \sqrt{L^2 - r^2\phi^2}$ and the relative compression can be approximated with $\frac{\delta L}{L} \simeq \frac{r^2\phi^2}{2L^2} = \frac{1}{2}$. For example, for a bundle of radius $r = 1\mu$m, length $L = 10\mu$m, twisted with a complete turn $\phi = 2\pi$, with pairs separated at $\delta\phi = 5^\circ$ the shift between the adjacent filaments is approximately 100nm and the relative length compression is $\delta L/L = 1\%$. We can test the twisting slide formula, Eq.(7). Since a uniform helix is produced by an infinitesimal bending at the base circle, by consider Eq.(3) with $R = a$, $L = a\cos\alpha$ we obtain $\delta_{\text{bend infinitesimal}} = La/R_0 = a\cos(\pi/2 - \alpha) = \delta_{\text{twist}}$. Within any 3-d deformation of a dynamic filament bundle, some twist among the filaments will occur. To date, the influence
of filament twisting has been neglected, possibly because the twist will often result ahead of or behind a region of the bending where the attention has been focused. A numerical analysis of twist generated in an active region and accumulated along the length of the axoneme is presented in [4]. For an axoneme of radius $r = 80\, \text{nm}$, linear separation between doublets $a = 40\, \text{nm}$, length $L = 20\, \mu\text{m}$ and total twist $\phi = 0.2\, \text{rad}$, Eq. (7) results in a sliding $\delta_{\text{twist}} = 30\, \text{nm}$ which is in good agreement with other numerical models, and experiments [4]. In this section we considered that filaments remain parallel while twisting, and consequently are confined in a cylindric surface. This simplifying hypothesis is revised in Section 3 and Eq.(7) is substituted with a formula valid for twisting around variable geometry bundle. However, even if the filaments begin to taper, splay, or intertwine, [15,35], hence loose parallelism, Eq.(7) can still give a close approximate evaluation of the situation.

### 3.2 Generalized twisting. Arbitrary helix

The bundle shape may change in time in response to the collective internal and external forces, such as in the case of T. brucei where the flagellum is wound around the cell as a variable radius-variable pitch helix [1,23,26]. In the following, we extend Eq.(7) for uniform sliding of a cylindrical helix to general twisting deformation when the filament bundle is itself deformed. Let $\Gamma$ curve be the central filament of this bundle described by an equation $\vec{r}_\Gamma(\alpha)$ having its Serret-Frenet trihedron given by $\vec{T}(\alpha)$ (the unit tangent vector), $\vec{N}(\alpha)$ (the principal normal vector) and $\vec{B}(\alpha)$ (the binormal vector), and metrics $G(\alpha) = \partial\vec{r}_\Gamma/\partial\alpha \cdot \partial\vec{r}_\Gamma/\partial\alpha$ [30]. In order to twist the filaments around the central filament we construct, for every $\alpha$, a circle of radius $r(\alpha)$ centered in $\vec{r}_\Gamma(\alpha)$, and parallel to the principal normal plane of $\Gamma$ at $\alpha$. Each such circle is parameterized by a new variable $\phi_p$ measuring the local twist of the pair at $\alpha$, around the local $\Gamma$ axis. The surface generated by this family of circles is $\vec{c}(\alpha, \phi_p) = \vec{r}_\Gamma(\alpha) + r(\vec{N}(\alpha)\sin\phi_p - (\vec{B}(\alpha)\cos\phi_p))$. In order to construct such a variable helix, we have to relate the $\alpha$ and $\phi_p$ parameters. The local (infinitesimal) height along this variable helix is equal to the corresponding infinitesimal element of the length of the supporting curve $\Gamma$, that is $ds_\Gamma = bd\phi_p$ where $b$ is the local pitch of this infinitesimal helix. Then, the variable helix $\gamma$ makes a constant angle with the tangent to the central filament curve $\Gamma$, namely $\tan \psi = b$. It results in the following relation between $\phi_p$ and $\alpha$: $\phi_p(\alpha) = \frac{1}{b} \int_0^\alpha G(\alpha') \, d\alpha'$, which provides the metrics of the variable helix

$$g(\alpha) = G(\alpha) \left[ \left( 1 - rk_\Gamma \sin(\phi_p(\alpha)) \right)^2 + r^2 \left( \tau_\Gamma + \frac{1}{b} \right) \right].$$

(8)

Here $k_\Gamma$ and $\tau_\Gamma$ are the curvature and the torsion of the $\Gamma$ central filament, respectively. The parameter $\alpha$ of the $\Gamma$ curve measures the deformation of the whole bundle, and its maximum value at the end of the bundle is $\phi_b$. All filaments in the bundle are described by the metrics in Eq.(8), the difference being made by the initial angular shift in $\alpha$ at the beginning of the bundle. From Eq.(8) one can obtain the curvature and torsion of any
filament (γ curve), and then calculate its length at a given α. For any two such filaments the difference of their lengths at α = φ₀ is their relative sliding.

The above procedure can calculate the twisting slide for any shape, but in the following we present an explanatory example where the bundle has a helical shape of radius R and pitch B. The filaments lie on the external surface of the bundle. Locally, the central filament γ is an infinitesimal helix having its principal normal always parallel to the normal plane to the bundle surface. Consequently the curvature of the central filament, kγ, is equal to the normal curvature of the bundle surface, and consequently is bounded between the values of the principal curvatures k₁₂ = {1/r, r/(R² + B²)} of the bundle surface [29]. The curvature kγ can be approximated with

\[ k_γ \simeq \begin{cases} \frac{R}{R^2 + B^2} & \text{if } b > b_{\text{lim}} \\ \frac{r}{r + b} & \text{if } b < b_{\text{lim}}, \end{cases} \]  

where \( b_{\text{lim}} = \sqrt{\frac{(R^2 + B^2)r - Rr^2}{R}} \) is the critical value of the pitch of the filament. The relative sliding of the filaments can be calculated with good approximation by using Eqs.(3,8,9) by using again the fact that a local twist is equivalent to an infinitesimal bending. We denote the radius and the pitch of the bundle helix with R, B. The bundle is a cylinder of radius R twisted as a helix with total length \( L_b = \sqrt{R^2 + B^2} \phi_b \), where \( \phi_b \) is the total twist angle of the bundle. We substitute in Eq.(3) \( L \rightarrow \sqrt{g(\alpha)}d\alpha \) and \( \phi_0 \rightarrow \alpha \), with \( g(\alpha) \) from Eq.(8). With this notations, we can find the sliding within the γ pair by using Eq.(9).

\[ \delta_γ \simeq \delta \phi \cos \left( \frac{\delta \phi}{2} + \phi - \alpha \right) \begin{cases} \frac{r^2 R}{b} \sqrt{\frac{R^2 + B^2}{r^2 + b^2}} & \text{if } \frac{R^2 + 4B^2 - \frac{r^2}{b}}{r\sqrt{R^2 + 3B^2}} > 1, \frac{(R^2 + B^2 - Rr)r}{b^2 R} > 1 \\ \frac{r^2 R}{b} \sqrt{\frac{B^2 + 2B^2}{R^2 + B^2}} & \text{if } \frac{R^2 + 4B^2 - \frac{r^2}{b}}{r\sqrt{R^2 + 3B^2}} > 1, \frac{(R^2 + B^2 - Rr)r}{b^2 R} < 1 \\ \frac{r^2 R}{b} \sqrt{\frac{R^2 + B^2}{r^2 + b^2}} & \text{if } \frac{R^2 + 4B^2 - \frac{r^2}{b}}{r\sqrt{R^2 + 3B^2}} < 1, \end{cases} \]  

where \( \delta \phi \) is the angular separation between the filaments in the pair, and \( \phi \) is the angular coordinate of the pair around the circumference.

For example we take \( L = 12 \mu \) length of the flagellum, \( r = 0.5 \mu \), a separation between pairs of \( \delta \phi = \frac{\pi}{6} \), and a full twist of \( 2\pi \) around the cell body (helices with variable radius and total bending plus twisting sliding will be calculated in the next section), like in the case of \( T. brucei \). In the case of very twisted cell (auger shape) we choose \( b = \frac{12}{2\pi} \mu, R = 1 \mu, \) and \( B = \frac{12}{2\pi} \mu \). The pitches \( b, B \) are calculated from the helix equation \( \text{Height}_{\text{helix}} = b \alpha_{\text{max}} \). These parameters place us in the second row of formula Eq.(10). The maximum twisting sliding in this shape is \( \delta \geq 7 \text{nm} \) or \( \delta/L \geq 0.5 - 0.7\% \).

In the case of an elongated cell body, we have \( b = \frac{12}{2\pi} \mu, R = 6 \mu \), and \( B = \frac{6}{2\pi} \mu \) and consequently we have a maximum slide of \( \delta/L = 1\% \). The main sliding control parameters are \( R/r \) and \( B/R \). These results are in good agreement with Eq.(7) for a cylindrical helix with uniform twisting. Even for a very small curvature and extreme bending, \( R/r < 3/2 \), we can still apply the same Eq.(12). Such estimations show that strongly coupled bending and twisting produces small sliding effects (percentages of the bundle length), and this
sliding is not strongly dependent on the variable curvature (on the bending radius). Thus, in a swimming stroke, the terminal sliding oscillates between .5% and 3% which is still small compared to a bending without twist for the same length. An optimal combination between sliding and twisting could adapt the swimming regime of the cell to the external viscosity, by changing the pattern from helical to planar geometry \cite{6,7}.

From numerical calculations with different values for $r, b, R, B$ we noticed that the curvature of the flagellum is oscillating around the largest of $k_\Gamma = \frac{R}{R^2 + a^2}$ and $k_{\gamma_0} = \frac{r}{r^2 + b^2}$, that is the the bundle curvature, and the curvature of the same filament as a cylindrical helix. A filament has a maximum curvature when $k_\Gamma \simeq k_{\gamma_0}$, i.e. when there is some geometric resonance between the two helices. Consequently, the average sliding almost doubles in such a situation. When the geometric parameters that mimic the shape of a T. brucei go from a relaxed (elongated) position ($R = 10\mu, r = 1.5\mu, B = 30/2\pi\mu, b = 12/2\pi\mu$) towards an auger twisted position ($R = 5\mu, r = 1.5\mu, B = 6/2\pi\mu, b = 12/2\pi\mu$) the average sliding almost doubles, from 4\% to about 8\%, which may relate to the mechanism by which these cells can effectively migrate through host tissue.

4 Mixed deformations. Parallel filaments

Herein we introduce a general sliding formula for simultaneous bending and twisting in 3-dimensions. We construct the bundle starting from its central filament $\vec{r}_C(s)$ ($s$ is the arc length) and constructing a smooth family of circles of radius $\rho = \rho(s)$ all centered in $\vec{r}_C(s)$ and lying in the normal plane of the central filament at $s$. Each outer filament $i$ is described by a curve $\vec{r}_i(s_i)$, $i = 1, 2, \ldots, N$, intersecting each circle only once. No outer filament can return towards the initial point, that is $\vec{t}_C(s) \cdot \vec{t}_i(s) > 0$ for any $s$ and $i$. We choose two arbitrary filaments (1 and 2) initially separated by $a$ at $s_1 = s_2 = 0$, and calculate their relative sliding at $s = L, \delta(L)$. We also assume $a, \delta(L) << L$, Fig.7.

The normal plane of filament 1 at $s_1 = L$ (defined by $\vec{n}_1(L)$ and $\vec{b}_1(L)$) intersects filament 2 at some $s_2 = s^* \neq L$ producing a sliding along the tangent direction $\delta(L) = L - s^*$. Under the hypothesis of small separation of pairs compared to the length of the bundle we can expand $\vec{r}_2(s^*)$ in Taylor series around $s_2 = L$. The intersection condition between the normal plane and filament 2 becomes $\vec{n}_1(L)C_1 + \vec{b}_1(L)C_2 + \vec{r}_1(L) - \vec{r}_2(L) = -\vec{t}_2(L)\delta$, where $C_{1,2}$ are the coordinates of the intersection point in a local 2-d frame in the normal plane. In the approximation $\vec{t}_1(L) \simeq \vec{t}_2(L)$ the infinitesimal sliding becomes

$$\delta(L) = \Omega|_{s,a}(\vec{r}_2 - \vec{r}_1)_{s=L} \cdot \vec{t}_1(L),$$

(11)

where $\Omega$ is the antisymmetric part of the second order differential with respect to $s$ and $a$ defined as $\Omega|_{s,a} = (1 + s \frac{\partial}{\partial s}|_{s=a=0} + a \frac{\partial}{\partial a}|_{s=a=0} + a s \frac{\partial^2}{\partial s \partial a}|_{s=a=0})$. Technically, $\Omega$ is provided by the second-order antisymmetric terms in the Taylor expansion of Eq. (11) with respect to $s$ and $a$ around $(0,0)$. We need to take into account the second differential because the sliding produced by twisting is on order of magnitude smaller than the sliding produced
by bending. The total slide is obtained by integration of Eq. (11) along $s \in [0, L]$. The operator $\Omega$ is the second order prolongation of the infinitesimal translation generator in $s$ and $a$ acting on the filament bundle surface, [30], and the infinitesimal sliding is the local action of this operator on the $(\vec{r}_1 - \vec{r}_2) \cdot \vec{t}$ function. This model can be tested by some simple examples. In the case of a cylindrical helix, the sliding in Eq. (11) is identical with Eq. (7) for twisting. Also, for a circular bend, if we put $a = \delta \phi R$ and $\phi - \phi_0 = \pi/2$, Eq. (11) approaches Eq. (3) for bending in the limit $\delta \phi_0 \simeq \sin(\delta \phi_0)$.

5 Bending and twisting deformations. Non-parallel filaments

In this section we present a formula for the total sliding produced by simultaneous bending and sliding, for any type of geometry with all parameters variable. Of course such a formula accommodates non-parallel filament configurations, and approaches in the limiting situations all the results presented in the previous sections. We describe the filament bundle as a family of smooth (at least second order differentiable) curves $\vec{r}(s_\beta, \beta)$ each parameterized by its the arc length $s_\beta$ and by $\beta$ to label the family. For each such curve we describe its metrics $g(\alpha, \beta)$ and the infinitesimal arc length $ds = \sqrt{g} d\alpha$. There are two possible interpretation of this last parameter; (1) $\beta$ can describe the deformation of a certain filament, and hence $\beta$ can be related to the time; or (2) $\beta$ can describe the mapping of a (deformed) filament into its neighbor pair filament, so it would be related to separation and non-parallelism.

5.1 General sliding formula

For a given point $\alpha, \beta$ along one filament its infinitesimal displacement in both parameters variations is

$$\vec{d}r = \vec{t} \sqrt{g} d\alpha + (i\delta + \vec{n} \Delta + \vec{b} \Lambda) d\beta,$$

(12)

where $\{\vec{t}, \vec{n}, \vec{b}\}$ is the local Serret-Frenet trihedron of the filament. The first term in the RHS (proportional with displacement $d\alpha$ along each filament) describes the regular advancement of the point along the curve by increasing the arc length $s$. The three shifting functions $\delta(\alpha, \beta), \Delta(\alpha, \beta)$ and $\Lambda(\alpha, \beta)$ characterize the displacement of the position of a point, placed at a certain fixed distance $s(\alpha)$ from the base ($\alpha = 0$), when we go from one filament to another (modify $\beta$). They represent shifting of points as follows: $\delta$ is the shift along the tangent of the filament (sliding), so when we change $\beta$, and move from one filament to another this function measures the actual sliding at any point $\alpha$ of the filament during this transformation. The function $\Delta$ measures the shift along the principal normal of the filament, that is the separation of filaments in the bending plane. The last function $\Lambda$ measures the shift along the binormal, that is the relative displacement of filaments.
perpendicular on the bending plane and on the tangent to the filament. For example, in
a planar bending we have from Eq.(1) the interpretation of the functions in Eq.(12) in
terms of separation and deviation from parallelism, \( \Delta = r \delta \phi + n_{tan} \) (also for a cylindrical
helix) and \( \Lambda = n_{rad} \).

From the smoothness property of the mathematical curves that describe the filaments
we can use the symmetry of second order derivatives and obtain the dynamical equation
for the metrics \[37\]
\[
\frac{\partial g}{\partial \beta} = 2 \left( \sqrt{g} \frac{\partial \delta}{\partial \alpha} - g k \Delta \right).
\]
By differentiation with respect to \( \beta \) the equation for the arc length is
\( s(\alpha, \beta) = \int_{0}^{\alpha} \sqrt{g} d\alpha' \), and by using Eq.(13) we obtain
\[
\frac{\partial L(\alpha_{max}, \beta)}{\partial s} = \delta(\alpha_{max}, \beta) - \delta(0, \beta) - \int_{0}^{\alpha_{max}} k \Delta \sqrt{g} d\alpha.
\]
(14)
The deformations, bending and twisting, change just the shape of the filaments, and not
the total length of each filament, so we have the local conservation of the length with
respect to deformations (\( \frac{\partial \alpha}{\partial \alpha} \)). If we consider no sliding at the beginning of the bundle
(\( \delta(\alpha = 0) \)), we obtain for sliding the expression
\[
\delta(\alpha, \beta) = \int_{0}^{\alpha} \sqrt{g} k \Delta d\alpha' = \int k \vec{d}r \cdot \vec{n} ds.
\]
(15)
The full description of the 3-d shifting \( \delta, \Delta, \Lambda \) can be related to the geometry of the filament (curve completely described by the initial position and by the curvature \( k(\alpha, \beta) \)
and torsion \( \tau(\alpha, \beta) \), [29], through two partial integro-differential equations. Following the
theory of curve motion [37] we have
\[
\frac{\partial k}{\partial \beta} = \frac{\partial^{2} \Delta}{\partial s^{2}} + (k^{2} - \tau^{2}) \Delta + \frac{\partial k}{\partial s} \int_{0}^{s} k \Delta ds' - 2 \tau \frac{\partial \Lambda}{\partial s} - \Lambda \frac{\partial \tau}{\partial s},
\]
\[
\frac{\partial \tau}{\partial \beta} = \frac{\partial}{\partial s} \left[ \frac{1}{k} \frac{\partial \Lambda}{\partial s} + \tau \Delta \right] + \frac{\tau}{k} \left( \frac{\partial \Delta}{\partial s} - \tau \Lambda \right) + \tau \int_{0}^{s} k \Delta ds'ight] + k \tau \Delta + k \frac{\partial \Delta}{\partial s}.
\]
(16)
These equations are written in terms of the arc length \( s \), but it is easy to substitute it
with \( \alpha \) through the transformation \( ds = \sqrt{g(\alpha, \beta)} d\alpha \). With Eqs.(15,16) we can solve
the geometry (or kinematics, if \( \beta \) is time) problem of the filament bundle. The direct
problem consists in finding the shape of each filament in the bundle if we are given the full
set of three shifts: tangent and two transverse. Namely the functions \( \delta, \Delta, \Lambda \) depending
on \( \alpha \), the evolution along the filament, and \( \beta \), for each filament. For a 9+1 axoneme
for example, \( \alpha \) takes values between zero at the basal plane, and \( \alpha_{max}, s(\alpha, \beta) = L \) for
a prescribed length \( L \), and \( \beta = 1, 2, \ldots, 10 \) is integer number. Consequently, for given
functions \( \delta, \Delta, \Lambda \), Eqs.(15,16) can be integrated with respect to the unknown functions
\( g(\alpha, \beta), k(\alpha, \beta), \tau(\alpha, \beta) \), within the prescribed initial data. Next, knowing the metrics,
curvature and torsion we can integrate the fundamental equations of the differential ge-
ometry of curves [29,30], and obtain the curves \( \vec{r}(\alpha, \beta) \), that is the shapes of any filament.
in the bundle. Conversely, the same Eq.(15,16) can solve the inverse problem, that is: given the shape of all filaments (the curves and consequently their metrics, curvature and torsion) we can integrate the equations and obtain the distribution of all three shifts for any filament in any point. Such an example is illustrated in Fig.8.

Both directions of integration are possible (though tedious numerical calculations may be involved) because the dynamical system described by Eq.(16) (having as parameter \( \beta \) instead of time) is an integrable system belonging to the MKdV- or NLS-equation hierarchies [37]. Eqs.(15,16) allow us to find the shape compatible with any distribution of sliding and twisting, and conversely, for a given shape to obtain the distribution of sliding and twisting. If one can relate the motor activity with all the 3-d sliding and shifts in a one-to-one correspondence, this approach could help a better understanding of the dynamics of filament bundles.

To illustrate with a simple, we choose a slightly deformed cylindrical helix, such that the curvature and torsion can still be considered \( s \)-independent, having almost constant bundle radius (\( \Delta \simeq 0 \), but with filaments free to change their angular distribution in the cross section (non-parallel). We have \( \Lambda \simeq \delta \), and from Eqs.(16) it results that \( \frac{\partial^2 \Lambda}{\partial s^2} = 0 \), and hence \( \Lambda(s,\beta) = \Lambda_0(\beta)s + \Lambda_1(\beta) \). This means that for any filament in the bundle (any \( \beta \)) the shift along the helical axis (along the binormal unit vector \( \vec{b} \)) is constantly increasing/decreasing with a ratio depending from filament to filament. This linear variable shift is proportional to the pitch of the helix. Eqs.(15,16) are nonlinear in all variables, but if we consider unknown only \( \delta, \Delta, \Lambda \), or conversely in \( g, k, \tau \), they become linear. This partial linearity allows the evolution of geometry to follow the evolution of shifting/sliding, and the other way around. Since these linear equations are of order three we also expect high dispersion, which means that localized zones of high sliding will disperse and re-distribute along \( s \) in time or from filament to filament. For example, an oscillating distribution of sliding and transverse shifting will produce same oscillations in curvature and torsion, generating waves and helices. On the other hand, such self-organized oscillations of internally shifted filaments were described in previous 2-dimensional models [5]. Wavelike propagating shapes were obtained by modeling a Hamiltonian system, and special behavior (bifurcations, spontaneous oscillations) was identified as critical for the self-generation of wave patterns [20,25,28,31]. Such type of behavior, even presence of solitons, can be already predicted from the nonlinear structure of Eqs.(16), as we describe further in section 5.2 without any reference to any particular physical model.

In the following, we focus on the sliding eq.(15) and we calculate the relative separation vector \( \vec{dr} \) between the ends of two given filaments \( (i,j) \), that is \( \vec{dr}(s) = \vec{r}_i(s) - \vec{r}_j(s) = \vec{r}_{ij}(s), \vec{r}_{ij}(0) = \vec{r}_{ij0}, |\vec{r}_{ij0}| = a \), where \( a \) is the initial linear separation between these 2 filaments. During the displacement \( ds \) of the \( i \) filament the vector \( \vec{r}_i \) performs an infinitesimal rotation of angle \( d\phi = kds \) around the binormal (local bending), and a rotation of angle \( d\psi = \tau ds \) around the tangent (local twist). Thus, its variation reads
\[ d\vec{r}_i = (\hat{b} \times \vec{r}_i) d\phi + (\hat{t} \times \vec{r}_i) d\psi. \]

The differential equation governing \( \vec{r}_i \) vector is

\[ \frac{d\vec{r}_i}{ds} = \vec{\omega} \times \vec{r}_i, \quad \vec{\omega} = kb + \tau \hat{t}. \]  

(17)

with initial conditions \( \vec{r}_i(0) = \vec{r}_{i0} \), namely the structural position of the filament \( i \) in the initial cross section of the un-deformed bundle (the base circle). Eq.(16) represents a rotation which copies the Darboux motion of the normal unit vector, since we have \( d\vec{n}/ds = \vec{\omega} \times \hat{n} \), with the exception that the origin of the vector \( \vec{r} \) also translates along the central filament with the arc length \( s \) [30]. Eq.(16) is integrable and its solution has the form

\[ \vec{r}_i(s) = e^{\int_0^s \vec{\omega} ds'} \vec{r}_{i0}. \]  

(18)

where the exponential is defined in the exponential matrix operator, and \( \vec{\omega} \) is the dual tensor of the vector \( \vec{\omega} \), that is \( \hat{\omega}_{nm} = \epsilon_{nmp} \vec{\omega}_p \) with \( n, m, p = 1, \ldots, 3 \) and \( \epsilon_{nmp} \) being the Levi-Civita tensor. By using Eqs.(15,17) we obtain the most general sliding formula for a pair \((i,j)\) of filaments in a bundle described by the normal \( \vec{n} \) and curvature \( k \)

\[ \delta_{ij}(s) = (\vec{r}_{i0} - \vec{r}_{j0}) \cdot \int_0^s e^{\int_0^{s'} \hat{\omega} ds''} \cdot \vec{n}_i(s') k_i(s') ds'. \]  

(19)

We mention that there is no equivalent equation for general 3-d sliding in the literature, so we can compare Eq.(18) only with numerical results. As a general check, if we choose a plane curve (zero torsion and constant binormal vector) the integral \( \int \hat{\omega} ds \) reduces to a rotation of angle \( \theta = \int k ds \) about the Oz axis. The right-action of this matrix through the second dot product rotates the normal \( \vec{n}(s) \) back to its initial direction \( \vec{n}(0) \), so we have \( (\vec{r}_{i0} - \vec{r}_{j0}) \cdot \vec{n}(0) = \Delta = a \), as in the 2-d sliding formulas from literature.

We can use Eq.(18) to calculate and predict the relative sliding for different pairs in different configuration of simultaneous bending and twisting. We performed several numerical checks of consistency between Eq.(18) and the other expressions obtained in this article for the sliding, namely Eqs.(2,3,5,7,10,11), and we found a very good match for different geometries. For example a helix of curvature \( k = \frac{R}{R^2 + b^2} \) and torsion \( \tau = \frac{b}{R^2 + b^2} \) has \( \vec{\omega} = (0, 0, g^{-\frac{1}{2}}) \), so the only nonzero elements in the matrix are \( \hat{\omega}_{12} = -\hat{\omega}_{21} = -g^{-\frac{1}{2}} \), and the exponential of this matrix is a rotation matrix around the Oz axis. By using this rotation matrix, and a particular solution of Eq.(17) for a bundle of nine pairs, we can calculate from Eq.(18) the sliding at any point \( s \) of the bundle and for any shape described by the corresponding curvature \( k \) and normal vector \( \vec{n} \).

In general, this sliding analysis provides local and global information about the geometric constraints of the bundle. For example, if the total slide at the end of a given pair is zero, the global integral curvature of this curve should also be zero. Thus, sliding directly interacts with the dynamics.

For example, certain boundary conditions at the end of the pairs (like clamped ends) introduce restrictions in the class of admissible shapes. An interesting situation (which has not been mentioned in literature) occurs in the mixed bending and twisting case. For
pure bending the relative sliding of a pair in a bundle is constantly increasing versus the
length of the bent segment (also proportional to the bending angle). If we first twist the
un-deformed (rectilinear) bundle around its symmetry axis, and then we bend it exactly
in the same configuration as before, the resulting relative sliding of the same pair is much
smaller. The larger the twist, the smaller the slide, Fig.8. The explanation is simple,
the twisted pair follows alternatively segments inside the bending (positive sliding) and
outside the bending (negative sliding) and the total final slide is compensated to zero
almost. The sliding at the end of the pair is actually produced only by the last unfinished
turn of twist around the bundle axis. This result was verified with a powerful numerical
code [36] and the same behavior was confirmed. This fact may provide insight about
the induced twist in flagellum around the body of a trypanosome-like cell, or about
the propagation of helical flagellar beats. Also, the combination between bending and
twisting could work like a molecular gear shift: for the same bending deformation, more
twist reduces the amount of sliding (but increases torque).

The generalized sliding equation Eq.(18) is useful in a variational formulation for the
shape problem, and hence the calculated sliding distribution can be related to molecu-
lar motors activity and distribution for different optimal natural configurations. From
differential geometry [29], we can express as a functional of the filament unit tangent
vector and its derivatives. Consequently the sliding functional Eq.(18) can be expressed
in terms of derivatives of the filament equation only which, under the request
of minimum slide with constant arc length, provides an Euler-Lagrange minimal action
system

$$\frac{\partial \Omega}{\partial \tilde{\omega}} \left( -\frac{\partial \tilde{\omega}}{\partial x} \tilde{r} + \frac{\partial \tilde{\omega}}{\partial x} \tilde{r} + \frac{\partial \tilde{\omega}}{\partial x} \tilde{r} \right) + \tilde{\Omega} = 0, \tag{20}$$

where the dot product between terms is performed in the tensor contraction sense, and
where \( \Omega[\tilde{\omega}[\tilde{r}, \tilde{r}, \tilde{r}]] = \frac{d^2}{ds^2} \int k \tilde{\omega} ds \cdot \tilde{r}_0 \). This partial differential system is difficult to solve
since \([\tilde{\omega}, \frac{d}{ds} \tilde{\omega}] \neq 0 \) and the derivatives of the exponential matrix (and consequently its
formal Taylor series) cannot be expressed in a concise form, but we conjecture that the
helix provides a solution, by minimizing the total sliding.

5.2 2-d applications

The 3-d sliding equation Eq.(18) can be reduce to a simpler expression for 2-dimensional
bending, by choosing \( \tau = 0, \tilde{b} = cst. \), and \( \Lambda = 0 \). The 2-dimensional version is also in
agreement with the expressions of the 2-d bend for constant normal separation from the
literature \( \Delta = a \), that is \( \delta = a \int k ds \) [5,23,26,34,35]. Like Eqs.(16) in the 3-d case, we
can also obtain a nonlinear partial differential system of equations in curvature and in the
two deformations for 2-d

$$\frac{\partial^2 \Delta}{\partial s^2} + \frac{\partial k}{\partial s} \delta + k^2 \Delta - \frac{\partial k}{\partial \beta} = 0, \quad \frac{\partial \delta}{\partial s} = k \Delta. \tag{21}$$
As an application of the **inverse** problem for a 2-d system, we investigate planar waves propagating along the bundle that provide a traveling wave profile for the curvature. In Fig. 9 we present the waveform of the shape and curvature $g$, which induce periodic variation of the sliding $\delta$ and transverse shift $\Delta$. We note that the largest sliding and transverse separation occur when the curvature has its fastest variation along the bundle. In the right frame of Fig. 9 we present a similar analysis, but in the case of a kink soliton traveling along the bundle. The sliding, the separation, and the curvature change in synchronism, and they are maximum when the soliton has the fastest variation in the shape.

Conversely, one can use Eq. (20) for the **direct** problem. predict the shape of the bundle for a given sliding function. This would represent the problem of predicting waves and beats from hypotheses over the action and synchronism of motors. For example, we provide a sliding $\delta$ as a traveling kink, Fig. 10, that is a localized wave that flips over the state of motors. Both curvature and normal separation result in a localized shapes. In the bottom of Fig. 10, we present the resulting 2-d shape of the bundle, by integration of Eq. (20) and of the intrinsic differential equation of the curvature [29], which strongly resembles a ciliary beat pattern.

### 6 Conclusions

We describe the dynamics of axoneme-like filament bundles from the perspective of the relative sliding between filament pairs, in an arbitrary shape bundle, in order to understand and explain mechanisms of self-deformation. The equations obtained can be used in further modeling approaches and experimental studies in order to calculate force and torque distributions. The analysis of filament bundles could be placed in between differential curves and surface theories. This study reports six expressions for sliding: for bending in parallel or arbitrary geometry, Eqs. (3,5) for twisting Eqs. (7,10), and for arbitrary sliding involving simultaneous bending and twisting Eqs. (11,18). We begin by analyzing two basic types of bundle deformations, circular bending and uniform twisting. Then we generalize the bending sliding formula for arbitrary shape, by integration of the uniform sliding with variable parameters. We exemplify with distributions of sliding between filaments for planar waves, rigid rotation and helical motion. Similarly, we generalize the sliding produced by arbitrary twisting, but in this case the equations request numerical analysis. We obtain the formula for uniform twisting, and for twisting around a deformed shape, and we illustrate these formulas with numerical examples from helical, and trypanosome-like shapes. We also analyze the influence of non-parallelism between filaments for both bending and twisting. By using a functional differential formalism, we obtain general formula for the sliding produced by any 3-d shape, Eq. (18). This result can provide the sliding distribution in any segment of any pair, for a bundle of an arbitrary geometry, stationary or in motion. Based on the theory of motion of curves, we obtain
a differential equation which connects the curvature, the tangent sliding, and the transverse shift of the filaments. Based on this equation, we can predict the distribution of the sliding (and possibly of motor activity) for any given flagellar shape and motion. Conversely, through these equations we can predict shapes for any arbitrary distribution of motor activity, if this distribution can be related with the sliding, twisting and transverse shifting. We observed that the coupling of twisting and bending, significantly reduces the relative sliding.

Several applications of the obtained sliding expressions are in good agreement with present geometrical models [14,15,38,39], and dynamical models [2,3,17,23,26,35]. The results are also discussed form the global geometrical invariants point of view, like total integral curvature and length, and are compared to the Hamiltonian models of similar systems [5,20,28,34,40], as well as with nonlinear effects observed or predicted in the literature. The equations obtained for the distribution of sliding along and among the pairs can be used in further modeling, theoretical approaches and/or experimental studies in order to calculate force and torque distributions, and–starting form experimental observed shapes–to calculate and predict energy transfer between motors and pairs, and in general to analyze the dynamics of the flagellum. These conclusions expand our understanding of cellular self-propulsion using flagellum or hair-like systems, and enhance the analysis of bending and twisting waves that can generate swimming.

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Figure Captions

1. Fig.1. Sliding induced by the bending of nine equal length $L$ filaments distributed on a base circle around a central filament. The bending center is $O_c$, and the bending plane makes $\phi_0$ angle with $Ox$ axis. $O'$ and $R'$ are the bending center and radius of an outer filament.

2. Fig.2. Density plot of the sliding $\delta_{tan}$ versus arc length $s$ for a deformed bundle of 9 parallel filaments. From white to black, the sliding values range from maximum negative value to its maximum positive value, respectively. Upper left: Right helix. When the helix rotates the density waves travel along the $s$-direction. Upper right: Left helix. Lower left: 2-d sine wave, the pattern travel to the right. Lower right: Rotation of a rigid bundle around a point. The pattern in travels along the vertical axis.

3. Fig.3. Sliding values for five (out of nine) filaments in a circular bend versus the arc length $s$ of the bend. Continuous straight lines represent the total sliding (from 0 to the current $s$) if the filaments are parallel. The dotted lines represent the total sliding (0 to current $s$) of the same filaments in a non-parallel configuration. Thin oscillating curves represent the infinitesimal sliding at the corresponding $s$. Upper left frame (3a): tangential deviation from parallelism given by an oscillatory angular separation between filaments. Upper right (3b): uniformly increasing tangential deviation from parallelism. Lower left (3c): radial oscillating non-parallelism. Lower right (3d): both tangential and radial deviations from parallelism.

4. Fig.4. The thin continuous lines represent infinitesimal sliding of the 5 filaments in a parallel bundle with variable radius and variable pitch (bundle represented in top left corner of frame) versus $s$. The dotted lines show same sliding for coupling two types of non-parallelism: oscillations in radius and in angular separation.

5. Fig.5. The relative sliding between three adjacent filaments subjected to constant tangential deviation from parallelism in a circular bend, versus $s$. The bending direction is vertical downwards in the two circular sections. The sliding $\delta_{12}$, $\delta_{23}$ in the case of parallel filaments, are plotted with continuous line, while the sliding for tangentially oscillating filaments ($\delta_{12}$, $\delta_{23}$) is plotted with dotted line.

6. Fig.6. Uniform twisting deformation for a circular cylinder.

7. Fig.7. Geometry of relative sliding for a pair of filaments (1,2) in a general 3-d deformation of the bundle. The origins of the two tangents represent the points of same length $L$ along each of the filaments, and these points are joined by the $\vec{dr}$ vector. The intersection of the normal plane at $s_1 = L$ with filament 2 determines a point $s^*$ related to the sliding, $\delta = L - s^*$ (drawn with thicker line)
8. Fig.8. Maximum sliding between two neighbor filaments \((r = 2\mu, \delta\phi = 2\pi/14, \phi = 0)\) plotted versus arc length. The straight line is for a bend of radius \(R = 6\mu\) at \(\phi_0 = \pi/2\), Eq.(5). If the bundle is first twisted around its axis with \(2\pi, 4\pi, 8\pi\) or \(16\pi\) rad, and then bend with the same radius, we have different sliding: much smaller and oscillating. Smaller sliding is produced by larger twisting angle. The number of periods of sliding oscillation is given by the torsion angle divided by \(2\pi\).

9. Fig.9. Traveling waves along the bundle. Top: Curvature \(k\), tangent sliding \(\delta\) and filament separation in the normal direction \(\Delta\) versus the the arc length. Bottom: the shape of the bundle.

10. Fig.10. A soliton \((sech^2\) profile) in curvature travels along the bundle and produces a kink-soliton (tanh profile) in the sliding \(\delta\) distribution, a soliton \((sech^2)\) in the separation shift \(\Delta\), and a symmetric pattern of 2-d beats in the bundle.
