Supporting Information

The counterbend dynamics of cross-linked filament bundles and flagella R. Coy and H. Gadêlha

1 Filament-bundle elastohydrodynamics

The vector $r(s, t)$ describes the position of a point which is an arclength s, with $0 \le s \le L$, along the neutral central line of a 2D representation of a cross-linked filament bundle or flagellar axoneme at a time t, relative to the fixed frame $\{e_x, e_y\}$. The filament bundle diameter is given by the constant a. In the absence of external forces, the filament bundle centreline assumes a horizontal position along e_x . Defining α to be the angle between \hat{t} , the unit tangent vector to **r**, and the axis e_x , we have:

$$
\hat{\mathbf{t}} = \mathbf{r}_s = (\cos \alpha, \sin \alpha)
$$

$$
\hat{\mathbf{n}} = (-\sin \alpha, \cos \alpha)
$$

Here r_s denotes the derivative with respect to s. The internal shear force $f(s, t)$ acts tangentially and in opposite directions on the sliding filaments r_1 and r_2 , which are defined as follows:

$$
\mathbf{r}_1 = \mathbf{r} + \frac{a}{2}\hat{\mathbf{n}}
$$

$$
\mathbf{r}_2 = \mathbf{r} - \frac{a}{2}\hat{\mathbf{n}}
$$

1.1 Filament displacement

Let $S_1(s)$ and $S_2(s)$ be the respective arclengths of r_1 and r_2 . Thus we have:

$$
\frac{\partial S_1}{\partial s} = \left| \frac{\partial \mathbf{r}_1}{\partial s} \right| = \left| \mathbf{r}_s - \frac{a}{2} \dot{\alpha} \mathbf{r}_s \right| = 1 - \frac{a}{2} \dot{\alpha}
$$

$$
\frac{\partial S_2}{\partial s} = \left| \frac{\partial \mathbf{r}_2}{\partial s} \right| = \left| \mathbf{r}_s + \frac{a}{2} \dot{\alpha} \mathbf{r}_s \right| = 1 + \frac{a}{2} \dot{\alpha}
$$

Here $\dot{\alpha}$ denotes the derivate of α with respect to s. Let Δ_0 be the initial filament sliding displacement at the base (s = 0), and let $\Delta(s)$ be the filament sliding displacement at a point s along the filament bundle, defined as the total arclength difference between the upper and lower filaments:

$$
\Delta(s) = \Delta_0 + \int_0^s \frac{\partial S_2}{\partial s'} - \frac{\partial S_1}{\partial s'} ds'
$$

$$
= \Delta_0 + a \int_0^s \frac{\partial \alpha}{\partial s'} ds'
$$

$$
= \Delta_0 + a \left[\alpha(s) - \alpha(0) \right]
$$

1.2 Internal forcing and basal displacement considerations

Suppose the internal shear density $f(s)$ is linearly related to the filament displacement, with a constant elastic resistance k: $f(s) = k\Delta(s) = k[\Delta_0 + a(\alpha(s) - \alpha(0))]$. Hook's law is assumed to give the relationship between the internal shear forcing and the sliding displacement at the base, where κ_e is a Hookean spring constant, so that:

$$
-\int_0^L f(s') \, ds' = \kappa_e \Delta_0
$$

$$
\Leftrightarrow -kL\Delta_0 - ka \int_0^L [\alpha(s') - \alpha(0)] \, ds' = \kappa_e \Delta_0
$$

By rescaling s so that it is expressed in multiples of L :

$$
-akL\int_0^1 [\alpha(s') - \alpha(0)] ds' = (kL + \kappa_e)\Delta_0
$$

$$
\Leftrightarrow -\frac{kL}{kL + \kappa_e} \int_0^1 [\alpha(s') - \alpha(0)] ds' = \frac{\Delta_0}{a}
$$

Let $\gamma = kL/(kL+\kappa_e)$, and note that $\gamma = 1$ and $\gamma = 0$ correspond to zero basal sliding resistance and a clamped base ($\Delta_0 = 0$) respectively. This gives:

$$
f(s) = ka \left[-\gamma \int_0^1 [\alpha(s') - \alpha(0)] ds' + \alpha(s) - \alpha(0) \right]
$$

1.3 The contact force, N

The material in the filament bundle segment $(s, L]$ exerts a resultant contact force N on the filament bundle segment [0, s]. The resultant contact torque is $\mathbf{r} \times \mathbf{N} + \mathbf{M}$, where M is the resultant contact couple:

$$
\mathbf{M} = E\mathbf{r}_s \times \mathbf{r}_{ss} + \frac{a}{2}\hat{\mathbf{n}} \times \left(\int_s^L -f(s') \, ds' \right) \hat{\mathbf{t}} - \frac{a}{2}\hat{\mathbf{n}} \times \left(\int_s^L f(s') \, ds' \right) \hat{\mathbf{t}}
$$

$$
= E\mathbf{r}_s \times \mathbf{r}_{ss} + a \left(\int_s^L f(s') \, ds' \right) \mathbf{r}_s \times \hat{\mathbf{n}}
$$

The constant E is the elastic stiffness of the filament bundle. Define:

$$
F(s) = \int_s^L f(s') \, \mathrm{d}s'
$$

Assuming there is no external couple acting on the filament bundle, the moment balance equation for an equilibrium rod gives:

$$
\frac{\partial \mathbf{M}}{\partial s} + \mathbf{r}_s \times \mathbf{N} = 0
$$

In this case:

$$
\frac{\partial \mathbf{M}}{\partial s} = E \mathbf{r}_{ss} \times \mathbf{r}_{ss} + E \mathbf{r}_s \times \mathbf{r}_{sss} - a f \mathbf{r}_s \times \hat{\mathbf{n}} + a F \mathbf{r}_{ss} \times \hat{\mathbf{n}} + a F \mathbf{r}_s \times \hat{\mathbf{n}}_s
$$

= $E \mathbf{r}_{ss} \times \mathbf{r}_{ss} + a F \mathbf{r}_{ss} \times \hat{\mathbf{n}} + \mathbf{r}_s \times (E \ddot{\alpha} \hat{\mathbf{n}} - E \dot{\alpha} \dot{\alpha} \mathbf{r}_s - a f \hat{\mathbf{n}} - a \dot{\alpha} F \mathbf{r}_s)$

Therefore to first order in α :

$$
\mathbf{N} = (-E\ddot{\alpha} + af)\hat{\mathbf{n}} + \tau \mathbf{r}_s
$$

Here τ represents physical tension. Then we have:

$$
\mathbf{N}_s = (-E\ddot{\alpha} + a\dot{f} + \dot{\alpha}\tau)\hat{\mathbf{n}} + (\dot{\tau} + E\dot{\alpha}\ddot{\alpha} - \dot{\alpha}af)\mathbf{r}_s
$$

1.4 Force balance

From the equilibrium equations, the contact force per unit length balances with the external force acting upon the filament bundle:

$$
\mathbf{N}_s + \mathbf{f}_{\text{ext}} = 0
$$

In our case, we are considering immersion in a fluid with low Reynolds number. Therefore inertial forces can be neglected, and we have $f_{ext} = f_{vis}$, the viscous drag force. From resistive force theory, the viscous drag force per unit length exerted on the filament bundle is given by:

$$
\mathbf{f}_{\rm vis} = -\zeta_{\perp}(\hat{\mathbf{n}}.\mathbf{r}_t)\hat{\mathbf{n}} - \zeta_{\parallel}(\hat{\mathbf{t}}.\mathbf{r}_t)\hat{\mathbf{t}} \tag{1}
$$

Balancing the viscous and contact forces gives per unit length gives:

$$
(-E\ddot{\alpha} + a\dot{f} + \dot{\alpha}\tau)\hat{\mathbf{n}} + (\dot{\tau} + E\dot{\alpha}\ddot{\alpha} - \dot{\alpha}af)\mathbf{r}_s = \zeta_{\perp}(\hat{\mathbf{n}}.\mathbf{r}_t)\hat{\mathbf{n}} + \zeta_{\parallel}(\hat{\mathbf{t}}.\mathbf{r}_t)\hat{\mathbf{t}}
$$

\n
$$
\Rightarrow \frac{1}{\zeta_{\perp}}(-E\ddot{\alpha} + a\dot{f} + \dot{\alpha}\tau)\hat{\mathbf{n}} + \frac{1}{\zeta_{\parallel}}(\dot{\tau} + E\dot{\alpha}\ddot{\alpha} - \dot{\alpha}af)\mathbf{r}_s = \partial_t \mathbf{r}
$$
\n(2)

Note that $\partial_t \mathbf{r}_s = \hat{\mathbf{n}} \partial_t \alpha$. Taking the derivative of (2) with respect to s and equating components in the $\hat{\mathbf{n}}$ direction obtains an equation of motion in α :

$$
\frac{1}{\zeta_{\perp}}(-E\dddot{\alpha} + a\ddot{f} + \ddot{\alpha}\tau + \dot{\alpha}\dot{\tau}) + \frac{1}{\zeta_{\parallel}}\dot{\alpha}(\dot{\tau} + E\dot{\alpha}\ddot{\alpha} - \dot{\alpha}af) = \partial_t\alpha
$$
\n(3)

1.5 Inextensibility condition

The physical tension is determined by the inextensibility condition, $\frac{\partial}{\partial t}(\mathbf{r}_s \cdot \mathbf{r}_s) = 2(\partial_t \mathbf{r}_s) \cdot \mathbf{r}_s = 0$. From this the tangential component of $\partial_t \mathbf{r}_s$ is equal to zero; thus differentiating (2) with respect to s and considering the components in the r_s direction, obtains a differential equation for τ :

$$
\frac{1}{\zeta_{\perp}}(E\dot{\alpha}\ddot{\alpha} - \dot{\alpha}af - \dot{\alpha}\dot{\alpha}\tau) + \frac{1}{\zeta_{\parallel}}(\ddot{\tau} + \partial_{s}(E\dot{\alpha}\ddot{\alpha}) - \partial_{s}(\dot{\alpha}af)) = 0
$$

$$
\ddot{\tau} - \frac{\zeta_{\parallel}}{\zeta_{\perp}}(\dot{\alpha}\dot{\alpha})\tau + \left(\partial_{s}(E\dot{\alpha}\ddot{\alpha}) - \partial_{s}(\dot{\alpha}af) + \frac{\zeta_{\parallel}}{\zeta_{\perp}}(E\dot{\alpha}\dddot{\alpha} - \dot{\alpha}af)\right) = 0
$$

From this, for our boundary conditions and via perturbation methods it can be seen that τ is of order α. Thus simplifying (3) to first order in α, noting again that $f = k[\Delta_0 + a(\alpha(s) - \alpha(0))]$, and making the assumption that α is small, gives the governing equation:

$$
\frac{1}{\zeta_{\perp}}(-E\alpha_{ssss} + a^2 k \alpha_{ss}) = \partial_t \alpha \tag{4}
$$

We now non-dimensionalise by changing the length scale by L, the time scale by w^{-1} . Consider solutions of the form $\alpha(s) = \text{Re}\{\tilde{\alpha}(s)e^{-iwt}\}\text{, and define the sperm compliance parameter, }$

$$
Sp = L\left(\frac{\zeta_{\perp}w}{E}\right)^{1/4}
$$

and the sliding resistance parameter $\mu = a^2 L^2 k / E$, which represents the relative importance of the flagellum elastic rigidity compared with the elastic resistance k of the cross linking.

The non-dimensional equation of motion is:

$$
\tilde{\alpha}'''' - \mu \tilde{\alpha}'' = i \operatorname{Sp}^4 \tilde{\alpha}
$$

Let r_j for $j = 1, 2, 3, 4$ be the four roots of the equation $r^4 - \mu r^2 - i \text{Sp}^4 = 0$. This produces four values of r_j which are of the form $-a + bi, a - ib, c + id, -c - id$, and we have the spatial solution:

$$
\tilde{\alpha}(s) = \sum_{j=1}^{4} C_j \exp r_j s \tag{5}
$$

2 Derivation of proximally actuated filament-bundle dynamics

In the case where we consider a proximal sinusoidal actuation of the filament-bundle, the following boundary conditions, to first order in α , apply at the proximal end $s = 0$. These correspond to angular actuation and fixed position in the e_y direction respectively:

$$
\alpha(0, t) = G \cos(\omega t)
$$

$$
\partial_t y(0, t) = 0 \Rightarrow \frac{1}{\zeta_{\perp}} (E \ddot{\alpha}(0) + a \dot{f}(0)) = 0
$$

At the distal end in this case, the first order boundary conditions correspond to zero force and torque respectively:

$$
\mathbf{F}_{\text{ext}}(L) = 0 \Rightarrow -E\ddot{\alpha}(L) + f(L) = 0
$$

$$
M_{\text{ext}}(L) = 0 \Rightarrow E\dot{\alpha}(L) = 0
$$

By substituting $f(s,t) = k\Delta(s,t) = k[\Delta_0(t) + a(\alpha(s,t) - \alpha_0(t))]$ and $\alpha(s) = \text{Re}\{\tilde{\alpha}(s)e^{-iwt}\}$ into the above boundary equations, the following are obtained:

$$
\tilde{\alpha}(0) = G
$$

$$
\tilde{\alpha}'''(0) - \mu \tilde{\alpha}'(0) = 0
$$

$$
\tilde{\alpha}''(1) + \mu \gamma \int_0^1 \tilde{\alpha}(s') - \tilde{\alpha}(0) ds' - \mu(\tilde{\alpha}(1) - \tilde{\alpha}(0)) = 0
$$

$$
\tilde{\alpha}'(1) = 0
$$

Substituting (4) into the above equations gives four linear equations in the C_j constant coefficients for our solution $\alpha(s,t) = \text{Re}\left\{\sum_{j=1}^4 C_j e^{r_j s - it}\right\}$, with the r_j being the complex roots of the equation $r^4 - \mu r^2 - i \text{Sp}^4$ and $R_j = e^{r_j}$:

$$
\sum_{j=1}^{4} C_j = G
$$

$$
\sum_{j=1}^{4} C_j (r_j^3 - \mu r_j) = 0
$$

$$
\sum_{j=1}^{4} C_j \left(r_j^2 R_j + \mu \gamma \left(\frac{R_j - 1}{r_j} - 1 \right) - \mu (R_j - 1) \right) = 0
$$

$$
\sum_{i=1}^{4} C_j r_j R_j = 0
$$

These equations can be expressed in matrix form:

$$
\begin{pmatrix}\nC_1 & C_2 & C_3 & C_4\n\end{pmatrix}\n\begin{pmatrix}\n1 & r_1^3 - \mu r_1 & r_1^2 R_1 + \mu \gamma \left(\frac{R_1 - 1}{r_1} - 1\right) - \mu (R_1 - 1) & r_1 R_1 \\
1 & r_2^3 - \mu r_2 & r_2^2 R_2 + \mu \gamma \left(\frac{R_2 - 1}{r_2} - 1\right) - \mu (R_2 - 1) & r_2 R_2 \\
1 & r_3^3 - \mu r_3 & r_3^2 R_3 + \mu \gamma \left(\frac{R_3 - 1}{r_3} - 1\right) - \mu (R_3 - 1) & r_3 R_3 \\
1 & r_4^3 - \mu r_4 & r_4^2 R_4 + \mu \gamma \left(\frac{R_4 - 1}{r_4} - 1\right) - \mu (R_4 - 1) & r_4 R_4\n\end{pmatrix} = \begin{pmatrix}\nG \\
0 \\
0\n\end{pmatrix}
$$

2.1 Calculation of propulsive force

The total viscous drag force is calculated by integrating the viscous drag force per unit length, f_{vis} , along the length of the filament bundle:

$$
\mathbf{F}_{\rm vis} = \int_0^L \mathbf{f}_{\rm vis}(s, t) \, \mathrm{d}s
$$

Noting that $\frac{\partial}{\partial t} \mathbf{r} = (\frac{\partial x}{\partial t}, \frac{\partial y}{\partial t})$, we substitute using (1) to obtain:

$$
\mathbf{F}_{\text{vis}} = -\int_{0}^{L} \zeta_{\perp} \left(\frac{\partial x}{\partial t} (-\sin \alpha) + \frac{\partial y}{\partial t} \cos \alpha \right) \hat{\mathbf{n}} + \zeta_{\parallel} \left(\frac{\partial x}{\partial t} \cos \alpha + \frac{\partial y}{\partial t} \sin \alpha \right) \hat{\mathbf{r}} \, ds
$$

\n
$$
\Rightarrow \mathbf{F}_{\text{vis}}.\mathbf{e}_{x} = -\int_{0}^{L} \zeta_{\perp} \left(\frac{\partial x}{\partial t} (-\sin \alpha) + \frac{\partial y}{\partial t} \cos \alpha \right) (-\sin \alpha) + \zeta_{\parallel} \left(\frac{\partial x}{\partial t} \cos \alpha + \frac{\partial y}{\partial t} \sin \alpha \right) \cos \alpha \, ds
$$

Take $\zeta_{\parallel} = R \zeta_{\perp}$. Therefore:

$$
\mathbf{F}_{\text{vis}}.\mathbf{e}_x = \zeta_\perp (1 - \mathbf{R}) \int_0^L \frac{\partial x}{\partial t} (-2\sin \alpha^2 - \cos \alpha^2) + \frac{\partial y}{\partial t} \cos \alpha \sin \alpha \, ds
$$

We take the assumption that $\zeta_{\perp} = 2\zeta_{\parallel}$ for long slender rods [1]. Integrating over time and taking the average gives us the time averaged viscous force that the fluid exerts on the filament: the propulsive force \bar{F}_x exerted on the fluid by the filament is equal and opposite to this. Thus we have:

$$
\bar{F}_x = -(\mathbf{F}_{\text{vis}}.\mathbf{e}_x)_{\text{avg}} = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} \left\{ \frac{1}{2} \zeta_\perp \int_0^L \frac{\partial x}{\partial t} (2\sin\alpha^2 + \cos\alpha^2) - \frac{\partial y}{\partial t} \cos\alpha \sin\alpha \, \mathrm{d}s \right\} \, \mathrm{d}t
$$

Rescaling time by $2\pi/\omega$, x, y and s by L, defining $l_w = (E/w\zeta)$ ^{1/4} and relabelling all variables we obtain:

$$
\bar{F}_x = -(\mathbf{F}_{\text{vis}}.\mathbf{e}_x)_{\text{avg}} = \frac{\omega \zeta_{\perp}}{2\pi} L^2 \int_0^1 \int_0^1 \frac{\partial x}{\partial t} (2 \sin \alpha^2 + \cos \alpha^2) - \frac{\partial y}{\partial t} \cos \alpha \sin \alpha \, ds \, dt
$$

$$
= \frac{\omega \zeta_{\perp}}{2\pi} l_\omega^2 \mathbf{Sp}^2 \int_0^{2\pi} \int_0^1 \frac{\partial x}{\partial t} (2 \sin \alpha^2 + \cos \alpha^2) - \frac{\partial y}{\partial t} \cos \alpha \sin \alpha \, ds \, dt
$$

$$
= \frac{\omega \zeta_{\perp}}{2\pi} l_\omega^2 \Upsilon_x(\mathbf{Sp}, \mu, \gamma)
$$

3 Derivation of relaxation filament-bundle dynamics

The equation of motion, derived through force and torque balance:

$$
\frac{1}{\zeta_{\perp}}(-E\dddot{\alpha} + a\ddot{f}) = \frac{1}{\zeta_{\perp}}(-E\dddot{\alpha} + a^2k\ddot{\alpha}) = \partial_t\alpha
$$

Non-dimensionalising via $s = Ls'$ and $t = \frac{L^4 \zeta_L}{E}$ $\frac{d\zeta_{\perp}}{E}t'$, and relabelling s' as s and t' as t, obtains a simplified governing equation:

$$
-\dddot{\alpha} + \mu \ddot{\alpha} = \partial_t \alpha
$$

Separation of variables results in the following equation, involving the eigenvalue λ :

$$
r^4 - \mu r^2 - \lambda^4 = 0
$$

Using the assumptions that $\mu \geq 0$ and $\lambda > 0$, define for each eigenvalue λ_n and corresponding relaxation constant λ_n^4 :

$$
q_{1_n} = \sqrt{\frac{\sqrt{\mu^2 + 4\lambda_n^4} - \mu}{2}}
$$

$$
q_{2_n} = \sqrt{\frac{\sqrt{\mu^2 + 4\lambda_n^4} + \mu}{2}}
$$

The solution in the relaxation case is therefore given by:

$$
\alpha(s,t) = \sum_{n} a_n S_n(s) e^{-\lambda_n^4 t},
$$

with $S_n(s) = C_1 \sin q_{1n} s + C_2 \cos q_{1n} s + C_3 \sinh q_{2n} s + C_4 \cosh q_{2n} s$ for each mode n. For ease of notation when considering the boundary conditions, define:

$$
Q_{1n} = \sin q_{1n}
$$

\n
$$
Q_{2n} = \cos q_{1n}
$$

\n
$$
Q_{3n} = \sinh q_{2n}
$$

\n
$$
Q_{4n} = \cosh q_{2n}
$$

The boundary conditions given below correspond to the proximal end being fixed in position and clamped respectively:

$$
\partial_t y(0, t) = 0 \Rightarrow \qquad S_n'''(0) - \mu S_n'(0) = 0
$$

$$
S_n(0) = 0
$$

A further two boundary conditions decribe the force and torque free distal end of the filament bundle:

$$
\mathbf{F}_{\text{ext}}(L) = 0 \Rightarrow S_n''(1) + \mu \gamma \int_0^1 S_n(s') - S_n(0) \, ds' - \mu(S_n(1) - S_n(0)) = 0
$$

$$
M_{\text{ext}}(L) = 0 \Rightarrow S_n'(1) = 0
$$

Substituting $S_n(s)$ into the above results in a set of linear equations in the C_i , represented by the matrix equation $CM = 0$, where:

$$
M_n = \begin{pmatrix} 0 & -q_{1_n}^3 - \mu q_{1_n} & -q_{1_n}^2 q_{1_n} + (1 - q_{2_n}) \frac{\mu \gamma}{q_{1n}} - \mu q_{1_n} & q_{1_n} Q_{2_n} \\ 1 & 0 & -q_{1_n}^2 Q_2 + \frac{\mu \gamma q_{1n}}{q_{1n}} - \mu Q_2 + \mu - \mu \gamma & -q_{1_n} q_{1_n} \\ 0 & q_2^3 - \mu q_2 & q_2^2 Q_{3_n} + (Q_{4_n} - 1) \frac{\mu \gamma}{q_2} - \mu Q_3 & q_2 Q_4 \\ 1 & 0 & q_2^2 Q_4 + \frac{Q_3 \mu \gamma}{q_2} - \mu Q_4 + \mu - \mu \gamma & q_2 Q_3 \end{pmatrix}
$$

$$
\mathbf{C} = \begin{pmatrix} C_1 & C_2 & C_3 & C_4 \end{pmatrix}
$$

Note that for non-zero S_n solutions, the solvability condition $Det(M_n) = 0$ must be met.

4 Eigenvalue relationships

The following tables were obtained via the identification of single eigenvalues for different parameters using Wolfram Mathematica, and subsequent data fitting within MATLAB to obtain approximate analytical expressions for the values of relaxation constants within different regimes, for the clamped and fixed proximal filament-bundle end case. The RMSEs from the data fitting process are also listed.

4.2 $\gamma = 0, 0 \le \mu \le 100$

4.3 $\gamma = 1, 100 < \mu$

4.4 $\gamma = 0$, 100 $< \mu$

5 References

1. Lauga E, Powers TR. 2009 The hydrodynamics of swimming microorganisms. Rep. Prog. Phys. 72, 096601. (doi:10.1088/0034-4885/72/9/096601)