# Supplementary materials: the mechanical worm model

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Recall that our mechanical worm (MW) model used in the simulation portion of our study is constructed from a chain of spherical beads of radius $a$. Each bead, indexed by $n$, is centered at $\mathbf{Y}_n$, and has an orientation vector $\hat{\mathbf{t}}_n$. The vector $\hat{\mathbf{t}}_n$ is also used as the unit tangent to the worm's centerline. Each bead is also subject to several forces and torques which sum to zero at each moment in the dynamics,

$$\mathbf{F}_n^C + \mathbf{F}_n^H + \mathbf{F}_n^B = \mathbf{0} \quad (1)$$

$$\boldsymbol{\tau}_n^E + \boldsymbol{\tau}_n^C + \boldsymbol{\tau}_n^D + \boldsymbol{\tau}_n^H = \mathbf{0}. \quad (2)$$

In this Supplementary Materials, we describe each of the models used to compute each of these forces and torques.

## 1 Elastic torques: $\boldsymbol{\tau}^E$

We resolve the worm's passive response to changes in its centerline curvature by treating it as an elastic beam divided in $N-1$ segments of length $\Delta L$. Consider three consecutive beads labelled, $n-1$, $n$ and $n+1$ with orientation vectors $\hat{\mathbf{t}}_{n-1}$, $\hat{\mathbf{t}}_n$ and $\hat{\mathbf{t}}_{n+1}$ respectively. We assume that between beads $n-1$ and $n$, $\mathbf{t}$ is given by

$$\mathbf{t}_-(l) = \frac{\hat{\mathbf{t}}_n - \hat{\mathbf{t}}_{n-1}}{\Delta L} l + \hat{\mathbf{t}}_{n-1} \quad (3)$$

and

$$\mathbf{t}_+(l) = \frac{\hat{\mathbf{t}}_{n+1} - \hat{\mathbf{t}}_n}{\Delta L} l + \hat{\mathbf{t}}_n \quad (4)$$

between $n$ and $n+1$ for $l \in [0, \Delta L]$.

The bending moment $\mathbf{M}(l)$ of an elastic beam is provided by the constitutive relation [1]

$$\mathbf{M}(l) = K_b \mathbf{t} \times \frac{d\mathbf{t}}{dl} \quad (5)$$

where $K_b$ is the bending modulus. Inserting Eqs. (3) and (4) into Eq. (5), we find that between beads, $\mathbf{M}$ is constant and given by

$$\mathbf{M}_- = \frac{K_b}{\Delta L}\hat{\mathbf{t}}_{n-1} \times \hat{\mathbf{t}}_n \tag{6}$$

between beads $n-1$ and $n$ and

$$\mathbf{M}_+ = \frac{K_b}{\Delta L}\hat{\mathbf{t}}_n \times \hat{\mathbf{t}}_{n+1} \tag{7}$$

between $n$ and $n+1$, respectively. Since the chain is in equilibrium, the resulting torque on bead $n$ due to deflections of the segments is given by the jump in $\mathbf{M}$. Thus, the bending torques on bead $n$ are given by

$$\boldsymbol{\tau}_n^E = \mathbf{M}_+ - \mathbf{M}_- = \frac{K_b}{\Delta L}\hat{\mathbf{t}}_n \times (\hat{\mathbf{t}}_{n+1} + \hat{\mathbf{t}}_{n-1}). \tag{8}$$

## 1.1 Constraint Forces and Torques: $\mathbf{F}^C$ and $\boldsymbol{\tau}^C$

Constraint forces and torques on the beads are introduced to enforce the inextensibility of each of the $N-1$ links. When $\Delta L \to 0$ and $N \to \infty$, these forces and torque converge to the tension and shear forces experienced by a continuous beam.

The positions of two neighboring beads are related to the tangent vector by

$$\mathbf{Y}_{n+1} - \mathbf{Y}_n = \int_0^{\Delta L} \mathbf{t}(l)dl. \tag{9}$$

With the tangent vector between each beads $n$ and $n+1$ given by Eq. (4), Eq. (9) becomes

$$\mathbf{Y}_{n+1} - \mathbf{Y}_n = \frac{\Delta L}{2}(\hat{\mathbf{t}}_{n+1} + \hat{\mathbf{t}}_n) \tag{10}$$

for $n = 1, \ldots, N-1$. Eq. (10) relates the bead positions with their orientations and serves as the constraint used to determine the forces and torques on a neighboring pair of beads. Rewriting Eq. (10) as

$$\mathbf{g}_n = \mathbf{Y}_{n+1} - \mathbf{Y}_n - \frac{\Delta L}{2}(\hat{\mathbf{t}}_{n+1} + \hat{\mathbf{t}}_n) = \mathbf{0}, \tag{11}$$

the forces and torques on the beads $n$ due to constraints $\mathbf{g}_n$ and $\mathbf{g}_{n+1}$ are given by (in indicial notation)

$$F_{n;i}^C = \lambda_{n-1;j}\partial g_{n-1;j}/\partial Y_{n;i} + \lambda_{n;j}\partial g_{n;j}/\partial Y_{n;i} \tag{12}$$

$$\tau_{n;i}^C = \lambda_{n-1;l}\epsilon_{ijk}\hat{t}_{n;j}\partial g_{n-1;l}/\partial \hat{t}_{n;k} + \lambda_{n;l}\epsilon_{ijk}\hat{t}_{n;j}\partial g_{n;l}/\partial \hat{t}_{n;k} \tag{13}$$

where $n = 1, \ldots, N-1$. $\boldsymbol{\lambda_n}$ are the vector Lagrange multipliers and $\epsilon_{ijk}$ is the permutation tensor.

The values of $\boldsymbol{\lambda_n}$ are determined iteratively each time-step. At the beginning of each iteration, the initial values of $\boldsymbol{\lambda}_n$ are either those from the previous iteration, or extrapolated from the values at the three previous time-steps,

$$\boldsymbol{\lambda}_n^{init} = 3\boldsymbol{\lambda}_n^{i-1} - 3\boldsymbol{\lambda}_n^{i-2} + \boldsymbol{\lambda}_n^{i-3}. \tag{14}$$

With the initial values for the Lagrange multipliers, the constraint forces and torques are computed, as are the other forces and torques experienced by the beads. The motion of the beads is then determined as are the resulting positions and orientation vectors. We then check that these new positions and orientations satisfy the constraints Eq. (11). In the simulations, we set our tolerance levels to keep the deviation in link length below $3.1 \times 10^{-4}\Delta L$. If the constraints are satisfied, the values are accepted, and time is advanced. If the constraints are not satisified, we determine new values for $\boldsymbol{\lambda}_n$ from the deviation $\boldsymbol{\epsilon}$ in the constraints and the initial values for $\boldsymbol{\lambda}_n$. Given the $2N-2$ linear constraints established by Eq. (11) for planar motion and the linear dependence of the bead motion on the applied forces and torques, the exact values of $\boldsymbol{\lambda}_n$ can be found from

$$\lambda_n = \lambda_n - \sum_{m=1}^{2N-2} (\partial \mathbf{g}_m / \partial \boldsymbol{\lambda}_n)^{-1} \epsilon_m. \tag{15}$$

Instead, to avoid computing $\partial \mathbf{g}_m / \partial \boldsymbol{\lambda}_n$, we use Broyden's method [2] and determine the values of $\boldsymbol{\lambda}_n$ iteratively. Broyden's method is a generalized secant method which updates an approximate Jacobian, $\mathcal{Q}$, as well as $\boldsymbol{\lambda}_n$ at each iteration. Once the suitable values of $\boldsymbol{\lambda}_n$ are determined and the constraints are satisfied, the time-step is accepted and the process is repeated.

## 2 Driving torques: $\boldsymbol{\tau}^D$

In our simulations, the worm's active muscular contractions are represented by a propagating wave of torques provided by a preferred curvature model [3]. In this model, the torques result from a deviation in the centerline curvature from

$$\kappa(s,t) = -\kappa_0(s)\sin(ks - 2\pi f t) \tag{16}$$

with $s \in [0, L]$. To replicate the higher curvature near the head of *C. elegans* observed during swimming, we take $\kappa_0(s)$ to be of the form

$$\kappa_0(s) = \begin{cases} K_0, & s \le 0.5L \\ 2K_0(L-s)/L, & s > 0.5L. \end{cases} \tag{17}$$

To obtain the driving torque on bead $n$, $\boldsymbol{\tau}_n^D$, we assume that the preferred curvature is constant between beads. The driving torque, therefore, results from jumps in the value at the bead positions multiplied by the worm's bending modulus. Accordingly, $\boldsymbol{\tau}_n^D$ is then given by

$$\boldsymbol{\tau}_n^D = K_b(\kappa(s_n,t) - \kappa(s_{n+1},t)) \tag{18}$$

where $s_n = (n-0.5)\Delta L$ and $n = 1,\ldots,N-1$.

# 3 Barrier Force: $\mathbf{F}^B$

In addition to the hydrodynamic interactions between the worm in the obstacles, we include in our model a pairwise repulsion force of the form

$$\mathbf{F}_{nm}^B = \begin{cases} -\frac{F_{ref}}{a+R}\left(\frac{R_{ref}^2-|\mathbf{Y}_n-\mathbf{Y}_m|^2}{R_{ref}^2-(a+R)^2}\right)^4(\mathbf{Y}_n-\mathbf{Y}_m), & |\mathbf{Y}_n-\mathbf{Y}_m| \leq R_{ref} \\ 0, & |\mathbf{Y}_n-\mathbf{Y}_m| > R_{ref} \end{cases} \tag{19}$$

with $R_{ref} = 1.1(a+R)$ and $F_{ref} = 114K_b/L^2$. Not only does this force prevent the beads in the chain from overlapping the obstacles, but provides the contact force experienced by the worm when it touches the micro-pillars.

# 4 Hydrodynamic Forces and Torques: $\mathbf{F}^H$ and $\boldsymbol{\tau}^H$

The force and torque balance for each bead establish a low Reynolds number mobility problem whose solution provides the velocity, $\mathbf{V}_n$, and angular velocity, $\boldsymbol{\Omega}_n$, for each bead. To solve this mobility problem, the force-coupling method (FCM) [4, 5]. In FCM, each particle $n$ is represented as a finite-force multipole expansion in the Stokes equations which is truncated after the force dipole term. Specifically, we have

$$\boldsymbol{\nabla} p - \eta\nabla^2\mathbf{u} = \sum_{n=1}^{N}\mathbf{F}_{tot}^n\Delta_n(\mathbf{x}-\mathbf{Y}_n) + \mathbf{G}^n\cdot\boldsymbol{\nabla}\Xi_n(\mathbf{x}-\mathbf{Y}_n) \tag{20}$$

$$\boldsymbol{\nabla}\cdot\mathbf{u} = 0 \tag{21}$$

where

$$\Delta_n(\mathbf{x}) = (2\pi\sigma_{n,\Delta}^2)^{-3/2}\mathrm{e}^{-r^2/2\sigma_{n,\Delta}^2}, \tag{22}$$

$$\Xi_n(\mathbf{x}) = (2\pi\sigma_{n,\Xi}^2)^{-3/2}\mathrm{e}^{-r^2/2\sigma_{n,\Xi}^2}. \tag{23}$$

The length scales $\sigma_{n,\Delta}$ and $\sigma_{n,\Xi}$ are related to the radius of bead $n$, $a_n$, through $a_n = \sqrt{\pi}\sigma_{n,\Delta} = \left(6\sqrt{\pi}\right)^{1/3}\sigma_{n,\Xi}$. In Eq. (20), $\mathbf{F}_{tot}^n = \mathbf{F}_n^C + \mathbf{F}_n^B$ is the total external force on bead $n$ and the antisymmetric part of the tensor $\mathbf{G}^n$ is related to the torque on the bead $\boldsymbol{\tau}_{tot}^n = \boldsymbol{\tau}_n^{bend} + \boldsymbol{\tau}_n^C + \boldsymbol{\tau}_n^D$ through $(G_{ij}^n - G_{ji}^n)/2 = \frac{1}{2}\epsilon_{ijk}\tau_{tot,k}^n$. The symmetric part of $\mathbf{G}^n$ is chosen so that

$$\int \frac{1}{2}\left(\boldsymbol{\nabla}\mathbf{u} + (\boldsymbol{\nabla}\mathbf{u})^{\mathrm{T}}\right)\Xi_n(\mathbf{x} - \mathbf{Y}_n)d^3\mathbf{x} = \mathbf{0}. \tag{24}$$

In the simulations, we obtain the flow field $\mathbf{u}(\mathbf{x})$ by solving the Stokes equations Eqs. (20) in a triply period domain of size $3q \times 3q \times 2.08R$ using a Fourier spectral method. For each case, the grid spacing is $dx = 2\sigma_\Xi(a)/3$ where $\sigma_\Xi(a)$ is the envelope size for the dipole Gaussian associated with a bead comprising the worm.

After obtaining the flow field $\mathbf{u}(\mathbf{x})$, the velocity and angular velocity of each bead $n$ are determined from

$$\mathbf{V}_n = \int \mathbf{u}(\mathbf{x})\Delta_n(\mathbf{x} - \mathbf{Y}_n)d^3\mathbf{x} \tag{25}$$

$$\boldsymbol{\Omega}_n = \frac{1}{2}\int \boldsymbol{\omega}(\mathbf{x})\Xi_n(\mathbf{x} - \mathbf{Y}_n)d^3\mathbf{x}. \tag{26}$$

In Eq. (26), $\boldsymbol{\omega}$ is the vorticity of the fluid.

With FCM, the resulting flow field for each bead is asymptotic to the Stokeslet, rotlet and stresslet fundamental solutions and provide the corresponding degenerate multipoles associated with these terms. The volume averaged integration captures the Faxén corrections for particle motion in a spatially varying flow field.

## References


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