Morphological transitions of axially-driven microfilaments

Yi Man and Eva Kanso

Aerospace and Mechanical engineering, University of Southern California, CA 90089

Supplemental Materials

We derived an elasto-hydrodynamic model of a filament driven by active force with an arbitrary force profile. The governing equations in dimensionless form is

$$\theta_t = -\theta_{ssss} - \Lambda\theta_{ss} - \left(1+\frac{1}{\gamma}\right)\Lambda_s\theta_s + 3\left(1+\frac{1}{\gamma}\right)\theta_s^2\theta_{ss} + \frac{1}{\gamma}f_{\parallel}\theta_s + \frac{\partial f_{\perp}}{\partial s}, \quad (1a)$$

$$\Lambda_{ss} - \gamma\theta_s^2\Lambda = 3\theta_{ss}^2 + (3+\gamma)\theta_s\theta_{sss} - \gamma\theta_s^4 + \frac{\partial f_{\parallel}}{\partial s} - \gamma f_{\perp}\theta_s. \quad (1b)$$

The boundary conditions for the filament with free-ends are given by the moment- and force-free conditions at both ends $s=0$ and $s=1$, leading to

$$\theta_s(0) = \theta_{ss}(0) = \theta_s(1) = \theta_{ss}(1) = 0, \quad (2a)$$

$$\Lambda(0) = \Lambda(1) = 0. \quad (2b)$$

We consider a force at $s = s_{\rm p}$ acting along the local tangential direction, with force profile given by a Dirac delta function,

$$f_{\parallel} = f_{\rm p}\delta(s - s_{\rm p}), \quad f_{\perp} = 0. \quad (3)$$

We discretize the arc length s uniformly into N segments and apply the second-order central difference formulae for all the derivatives of θ and Λ, in the bulk,

$$(X_s)_j = \frac{1}{2\Delta s}(-X_{j-1} + X_{j+1}), \quad (4a)$$

$$(X_{ss})_j = \frac{1}{\Delta s^2}(X_{j-1} - X_j + X_{j+1}), \quad (4b)$$

$$(X_{ssss})_j = \frac{1}{\Delta s^4}(X_{j-2} - 4X_{j-1} + 6X_j - 4X_{j+1} + X_{j+2}), \quad (4c)$$

where $\Delta s = 1/N$, $j = 2, 3...N$, and X represents either θ or Λ. At the boundaries, the discretization is

$$(X_s)_1 = \frac{1}{2\Delta s}(-3X_1 + 4X_2 - X_3), \quad (5a)$$

$$(X_{ss})_1 = \frac{1}{\Delta s^2}(2X_1 - 5X_2 + 4X_3 - X_4), \quad (5b)$$

$$(X_s)_{N+1} = \frac{1}{2\Delta s}(3X_{N+1} - 4X_N + X_{N-1}), \quad (5c)$$

$$(X_{ss})_{N+1} = \frac{1}{\Delta s^2}(2X_{N+1} - 5X_N + 4X_{N-1} - X_{N-2}). \quad (5d)$$

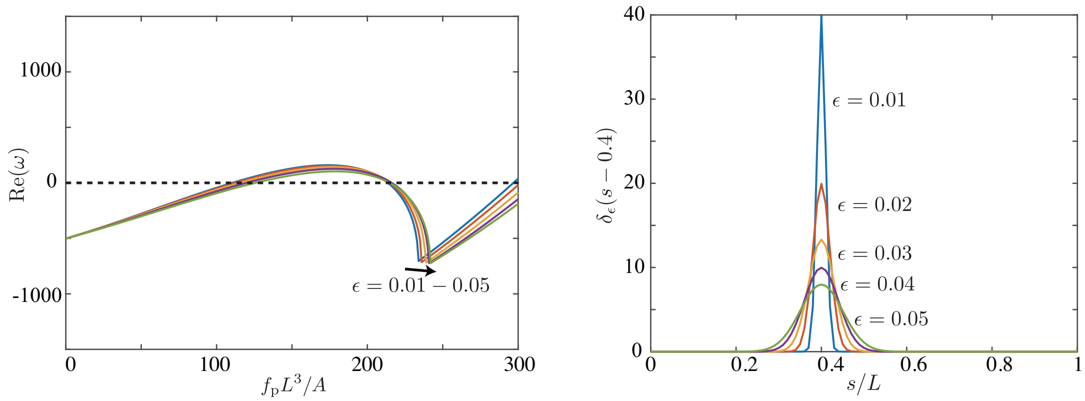

FIG. 1. Left: Real part of dominant eigenvalues when $s_\mathrm{p} = 0.4$, with regularization coefficient $\epsilon = 0.01 - 0.05$. Right: Regularized Dirac delta function with $\epsilon = 0.01 - 0.05$.

At each time step, we first calculate the tension Λ from (1b), then march (1a) in time with a modified Crank-Nicolson method. We treat the linear terms implicitly and the nonlinear terms explicitly. At time step k, the discrete equations are given by

$$\Lambda^k_{ss} - \gamma \left(\theta^k_s\right)^2 \Lambda^k = 3(\theta^k_{ss})^2 + (3+\gamma)\theta^k_s\theta^k_{sss} - \gamma(\theta^k_s)^4 + f_\mathrm{p}\frac{\partial\delta(s-s_\mathrm{p})}{\partial s} \tag{6a}$$

$$\begin{aligned}\frac{\theta^{k+1}-\theta^k}{\Delta t} =& -\frac{1}{2}\left(\theta^k_{ssss}+\theta^{k+1}_{ssss}\right) - \frac{1}{2}\left[\Lambda^k\left(\theta^k_{ss}+\theta^{k+1}_{ss}\right)\right] \\ & -\frac{1}{2}(1+\gamma^{-1})\left[\Lambda^k_s\left(\theta^k_s+\theta^{k+1}_s\right)\right] + \frac{3}{2}(1+\gamma^{-1})\left[\left(\theta^k_s\right)^2\left(\theta^k_{ss}+\theta^{k+1}_{ss}\right)\right] \\ & +\frac{1}{2\gamma}f_\mathrm{p}\delta(s-s_\mathrm{p})\left(\theta^k_s+\theta^{k+1}_s\right).\end{aligned} \tag{6b}$$

We use $N = 100$ in our simulations, the time step is around 10^{-4}. To avoid the singularity, the Dirac delta function is regularized using the regularization function

$$\delta_\epsilon(x) \approx \frac{1}{\sqrt{2\pi}\epsilon} e^{-\frac{x^2}{2\epsilon^2}}. \tag{7}$$

In Fig. 1, we calculate the eigenvalues for $s_\mathrm{p} = 0.4$ (shown in Fig. 5 of the main document) with regularization coefficient $\epsilon = 0.01 - 0.05$. Clearly, the instability features are not affected qualitatively by the exact value of ϵ. In the main document, we set $\epsilon = 0.01$ throughout.

We next choose a finer discretization $N = 200$ with $\epsilon = 0.01$. The results show the same level of accuracy, see Fig. 2.

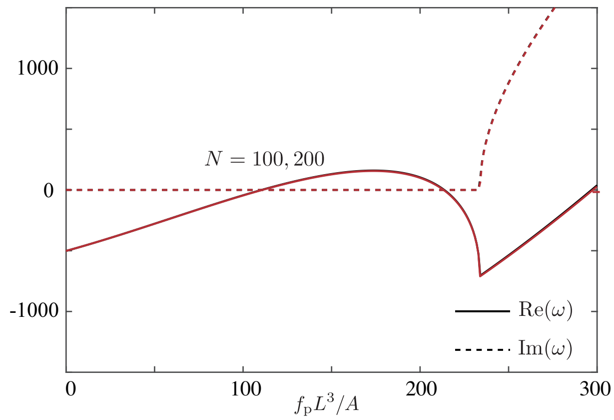

FIG. 2. Dominant eigenvalues when $s_{\mathrm{p}} = 0.4$, with regularization coefficient $\epsilon = 0.01$. Two sets of line overlap, with number of discretization $N = 100$ and 200 respectively.