IMPERIAL

Nonlinear Dynamics of Active Filaments

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Motivation

Active filaments are thin, elastic, slender rods that are commonly observed in nature. Driven by motor protein activity, active filaments play a crucial role in cellular processes such as **fluid transport**, **mixing**, and **swimming**, among many others.

Our goal is to analyse **filament dynamics in biological settings** using our numerical model, identify self-sustaining states (limit cycles), detect transitions between these states (bifurcations), and compute the stability of these states.

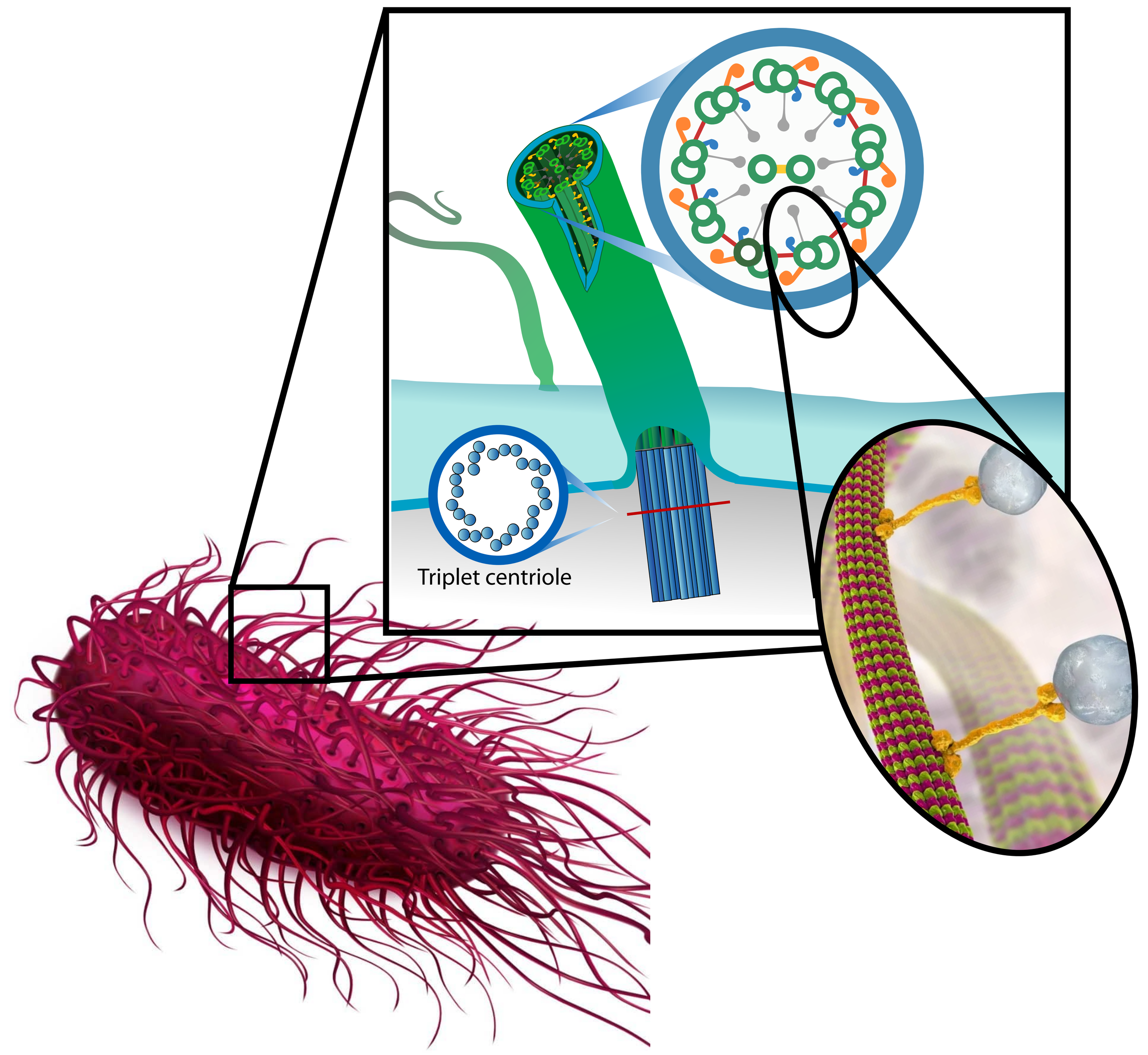

Figure 1: Illustration of a microfilament in a eukaryotic cell's flagella. Adapted from online illustrations of Mariana Ruiz Villarreal[3] and Kateryna Kon[4].

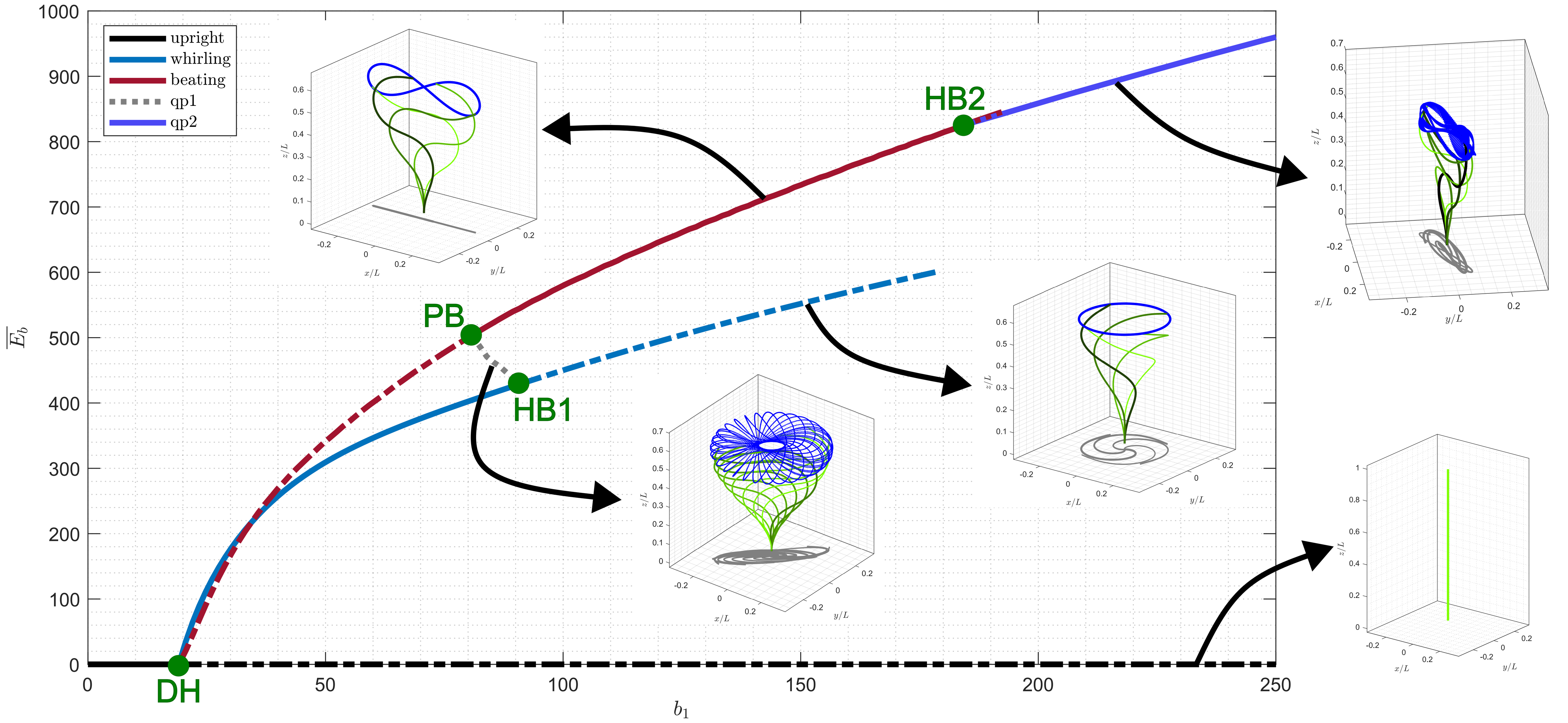

Figure 3: Bifurcation diagram for the squirming filament, average bending energy $(\overline{E}_b)$ vs. motor protein activity (b_1). Upright is a steady state. Whirling and beating are periodic states. QP1 is unstable and carries the characteristics of both whirling and beating. QP2 is stable and describes a coiled filament state with changing handedness. DH: double Hopf bifurcation, PB: pitchfork bifurcation, HB: Hopf bifurcation.

The Model and Methods

- Molecular motors exert compressive forces on the filament and create a slip-flow over filament surface.
- Discretise the filament into self-locomoting segments.
- Solve the equations in the Stokes limit[1]: velocity and forces are linearly related!
- Model the squirming effect (effect of motor proteins) as a nonlinear forcing and solve for the velocity using Faxén's Laws.[2]

$$\begin{bmatrix} \boldsymbol{V} \\ \boldsymbol{\Omega} \end{bmatrix} = \mathcal{M}^{\text{RPY}} \begin{bmatrix} \boldsymbol{F}^H \\ \boldsymbol{T}^H \end{bmatrix} + \mathcal{M}^{\text{sq}} \begin{bmatrix} \boldsymbol{H}(b_1) \\ 0 \end{bmatrix}$$

- b_1 measures **motor protein activity**.
- Analyse recurrent patterns in the dynamics using Poincaré maps.
- Use a Jacobian-free Newton-Krylov (JFNK) method to obtain accurate representations of periodic states and compute their Floquet stability.
- Track each solution branch to find the bifurcations.

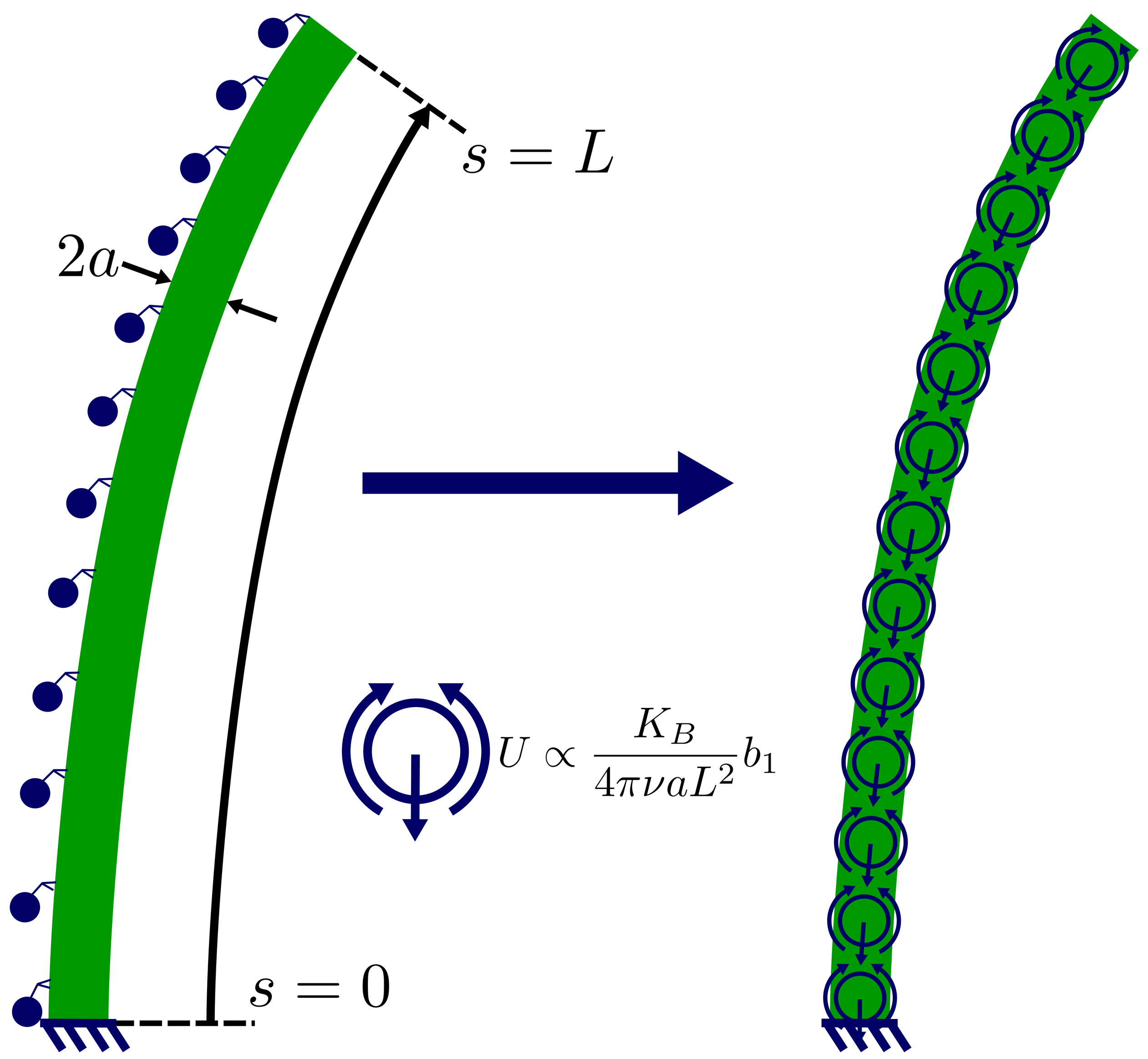

Figure 2: Schematic of the modelling approach employed to describe the motor protein activity and resulting filament dynamics numerically. The filament is discretised into self-locomoting squirmers. a is the radius of the filament's cross-section, L is the length of the filament, K_B is filament stiffness, and ν is fluid viscosity.

Table 1: Bifurcations of the squirming filament, with b_1 values given in the bottom row. DH: double Hopf bifurcation, PB: pitchfork bifurcation, HB: Hopf bifurcation.

Event	DH	PB	HB1	HB2
b_1	19.1	80.8	90.8	184

Results

We identify five distinct states: **upright**, **whirling**, **beating**, **QP1**, and **QP2**. Upright is steady; whirling and beating are periodic orbits; QP1 and QP2 are quasi-periodic states.

- **Double Hopf** bifurcation: a dynamic instability with two distinct eigenmodes. The phase difference between the modes determines the state: beating $(\Delta\phi = 0)$, and whirling $\left(\Delta\phi = \frac{\pi}{2}\right)$.
- **Bistability** of whirling and beating in the range $b_1 \in [80.8, 90.8]$.
- **Modal decomposition** of QP1 into whirling and beating: $\boldsymbol{u}_{QP1}(t) \approx c_W\, \boldsymbol{u}_W(t) + c_B\, \boldsymbol{u}_B(t + \phi)$, displaying both characteristics.
- At high actuation, transition to QP2 – a coiled filament with changing winding direction.
- **Robust dynamics** to changes in motor protein activity b_1. QP2 does not transition to chaos!

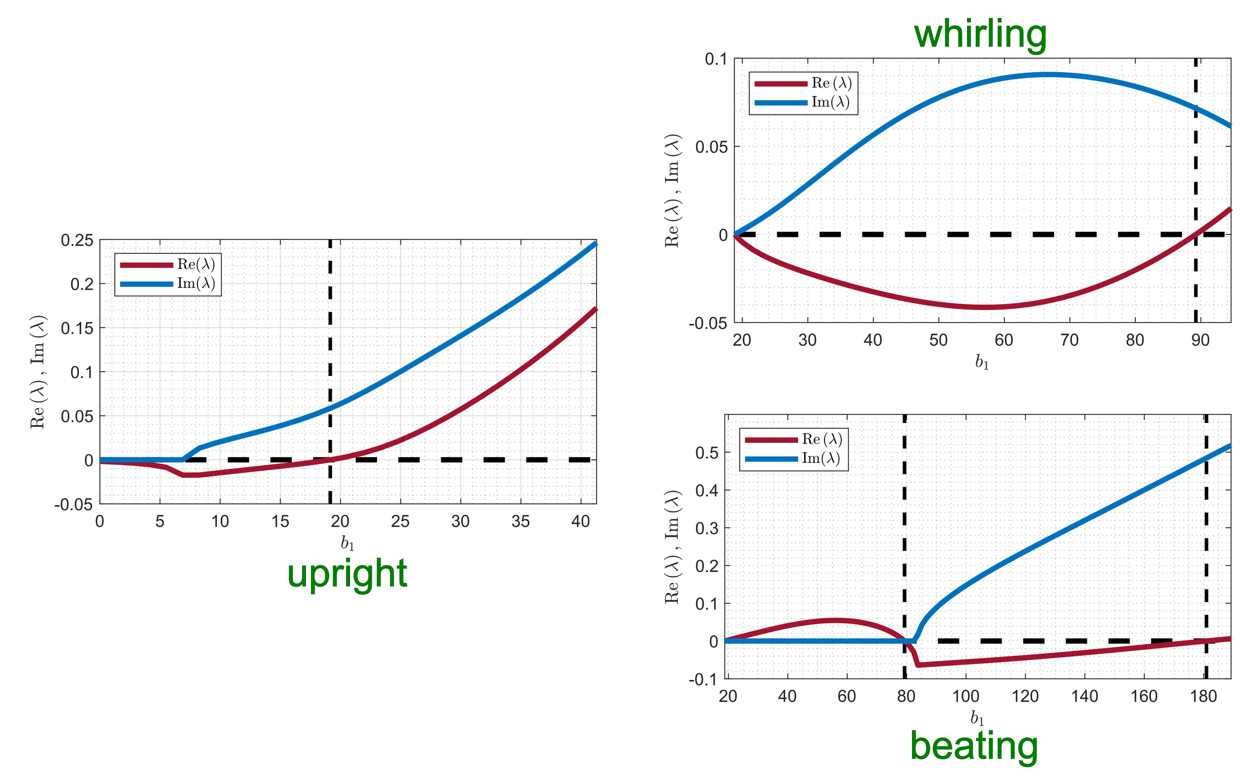

Figure 4: Linear stability analysis of the upright, whirling, and beating states: instability growth rate (λ) vs. motor protein activity (b_1).

Future Work

- Data-driven analysis of the dynamics to explain the hydrodynamic interactions leading to the observed filament behaviours.
- Extending the current framework to investigate collective dynamics of multiple filaments.

References

[1]Schoeller et al. JCP, 2020. [2]Clarke, B. PhD Thesis. [3]`http://ladyofhats.com/` [4]`https://www.sciencephoto.com/`

Affiliations

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