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Modelling Active Filaments using the Squirmer Model

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1. MOTIVATION

Microtubules are long, slender polymers, which form the basis of cilia and flagella. They undergo oscillations driven by dynein; a molecular motor which translocates along the microtubule's length. In cilia, this motion can coordinate to cause ciliary beating, for example allowing for propulsion of ciliated cells. By modelling the microtubule as a slender filament in low Reynolds number flow, our aim is to develop a model that accounts for this dynein-generated driving force and to understand and characterize the resulting microtubule motion.

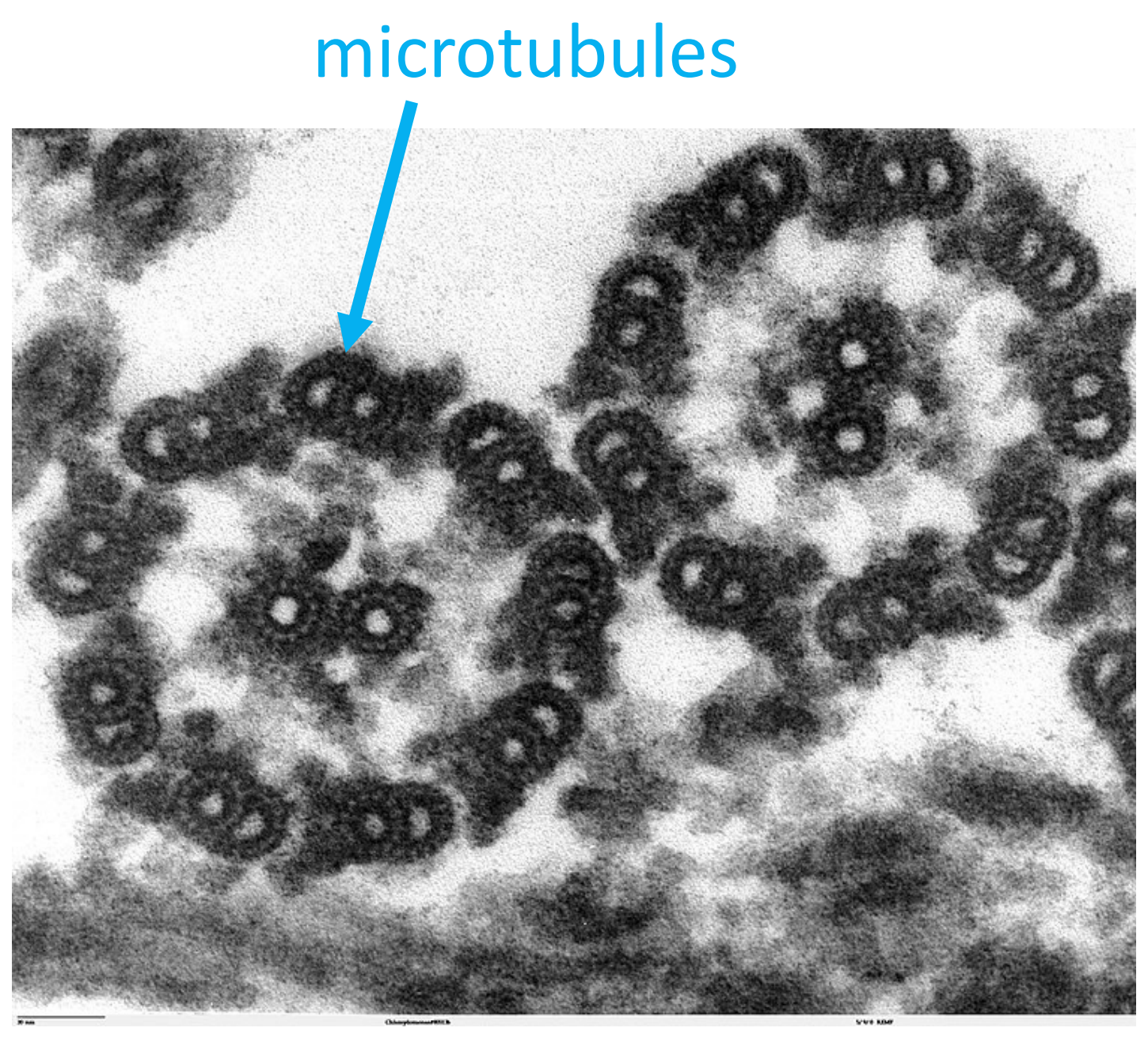


Figure 1: *A cross-section of two cilia from [1]. The small circular rings shown are microtubules, in a '9+2 arrangement'.*

2. THE MODEL

- Following similar modelling strategies to [2,3], we introduce a slip flow of strength B_1 along the length of the filament and discretise into N segments (see **Figure 2**).
- The model represents a continuous stream of molecular motors translocating along the filament length.

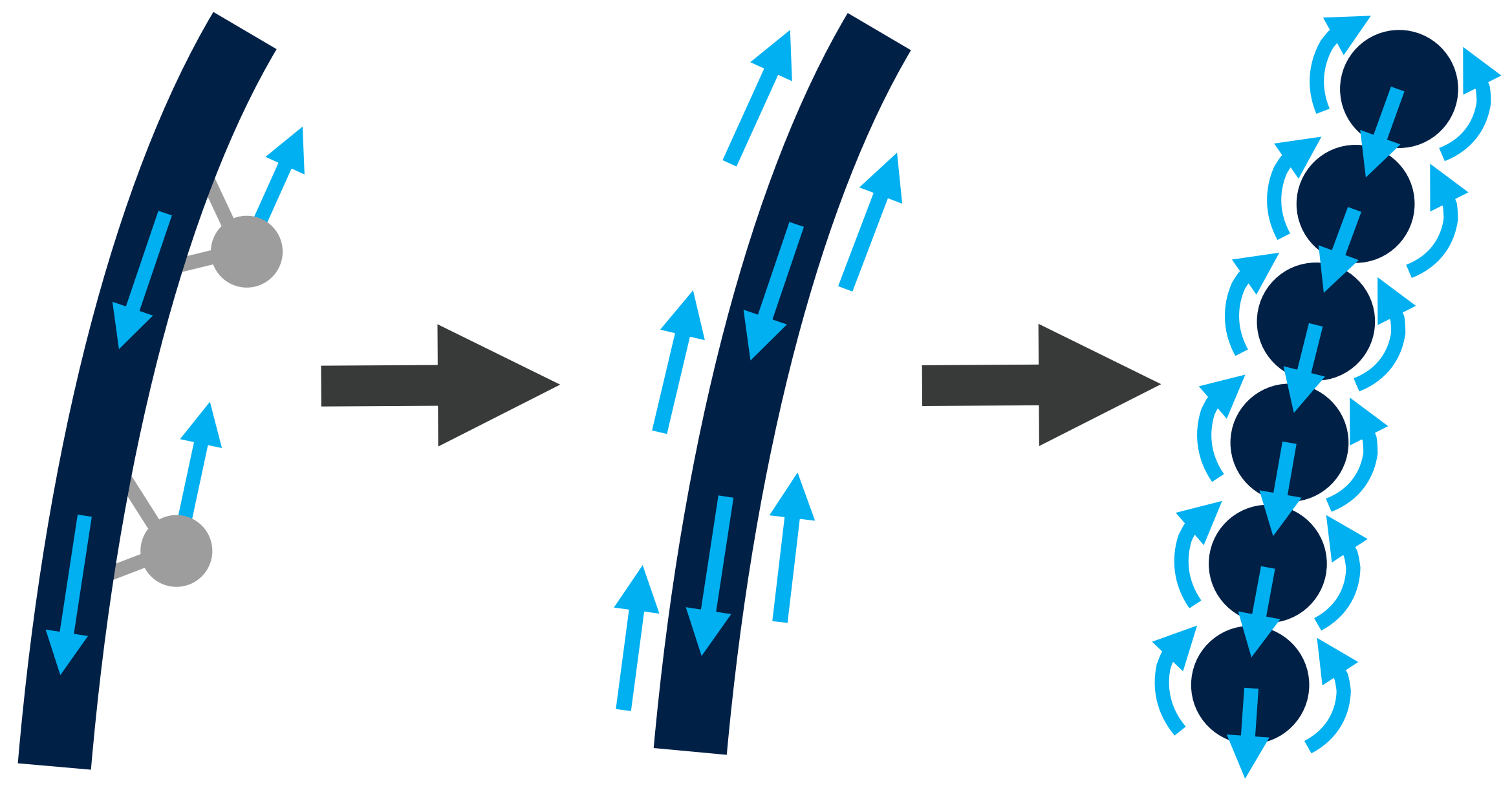


Figure 2: *A schematic of (left) the physical problem, (middle) our model in the continuous setting, (right) our model in the discrete setting.*

- Model filament as N segments, radius a.
- Segment n has position vector $\boldsymbol{x}_n$ and tangent $\hat{t}_n$. We impose a surface velocity $\boldsymbol{u} = B_1 \cos\theta$.
- For each segment we have force and torque balances:
$$F_C - F_H = 0$$
$$T_E + T_C - T_H = 0$$
where F_C/T_C are the constraint forces/torques to enforce inextensiblity of the filament, T_E are the elastic torques and F_H/T_H are the hydrodynamic force/torque, accounting for the effect of the fluid.

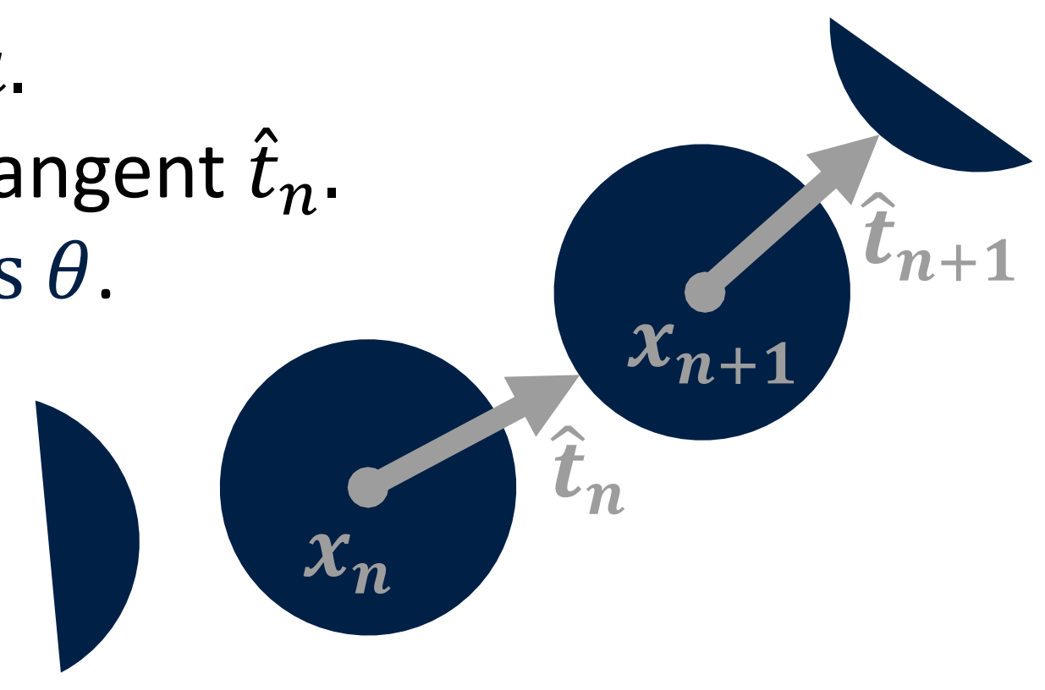


Figure 3: *Segments n and $n+1$ in our filament discretisation.*

- In Stokes flow, velocity and angular velocity of each segment are then found through the relation:
$$\begin{bmatrix} V \\ \Omega \end{bmatrix} = M \begin{bmatrix} F_H \\ T_H \end{bmatrix} + \boldsymbol{M^{active}} \begin{bmatrix} \boldsymbol{H(B_1)} \\ \boldsymbol{0} \end{bmatrix}$$
- Explicit approximations of M can be found. The blue term describes the effect of the slip velocity.
- Integrate the system forward in time to progress the simulation, using unit quaternions to describe the rotation of the local frame over time.
- B_1 controls the strength of the slip flow, which generates a compressive force in the $-\hat{t}$ direction. Hence strength of compressive force related to B_1.
- Non-dimensionalise: $\hat{\boldsymbol{B}}_{\boldsymbol{1}} = \boldsymbol{C}\boldsymbol{B}_{\boldsymbol{1}}$ where C depends on fluid viscosity, filament length and bending rigidity.
- **We vary $\hat{\boldsymbol{B}}_{\boldsymbol{1}}$ and observe the corresponding behaviours.**

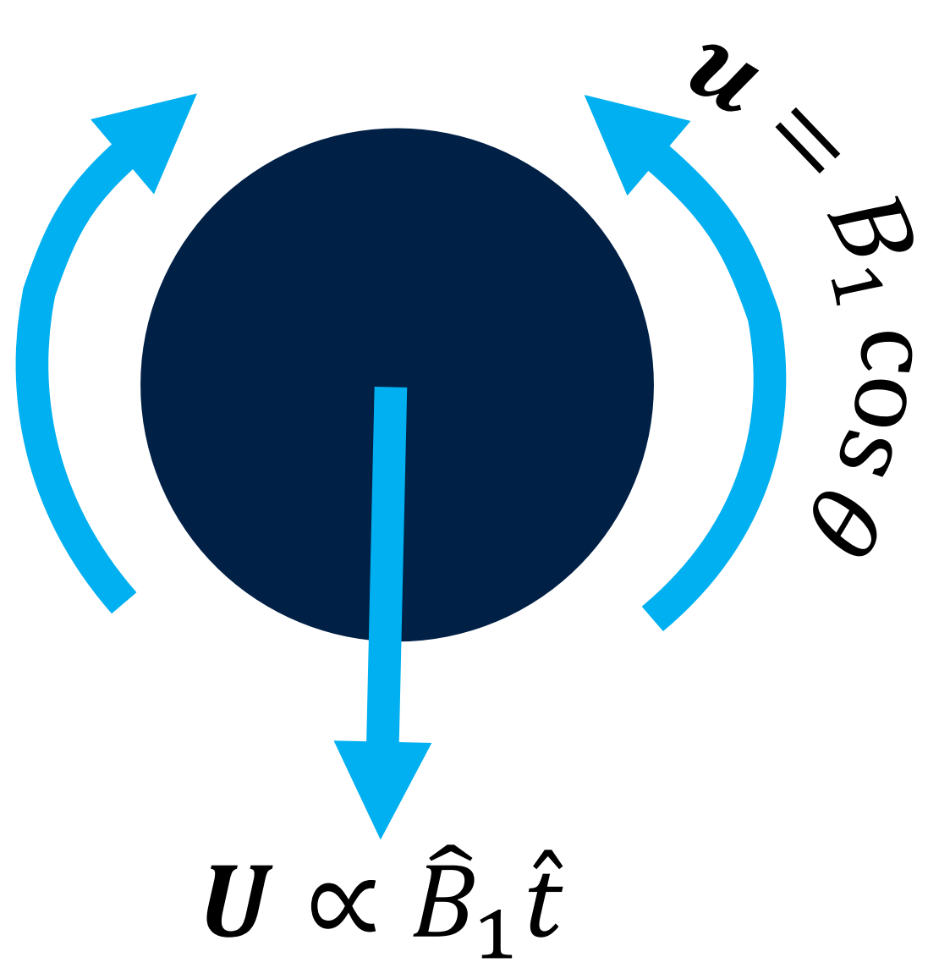


Figure 4: *The slip velocity on each segment generates a `swimming velocity' proportional to the non-dimensional forcing, $\hat{B}_1$.*

3. RESULTS – ONE FILAMENT

- We run simulations for one filament in both 2D/3D.
- In 2D, only see non-trivial behaviours for $\hat{B}_1$ above a critical value, $\hat{B}_1^C$ (see **Figure 5**).
- In 3D, the onset of oscillations again begins at $\hat{B}_1 = \hat{B}_1^C$.
- With increasing $\hat{B}_1$, we observe whirling, then a planar/transitioning region, before a coiling regime (see **Figure 6**).
- Surprising that coiling/whirling, which are physically similar, are separated by a distinct, planar regime.

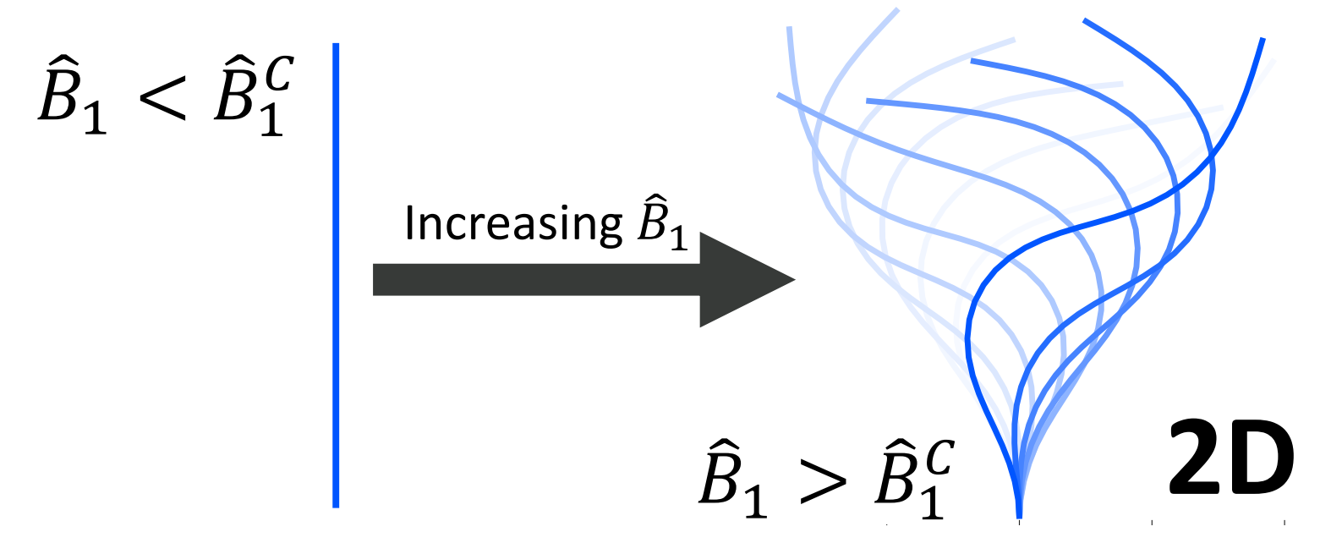


Figure 5 (left): *Snapshots of 2D simulations for two values of $\hat{B}_1$ on either side of the bifurcation point, $\hat{B}_1^C$.*

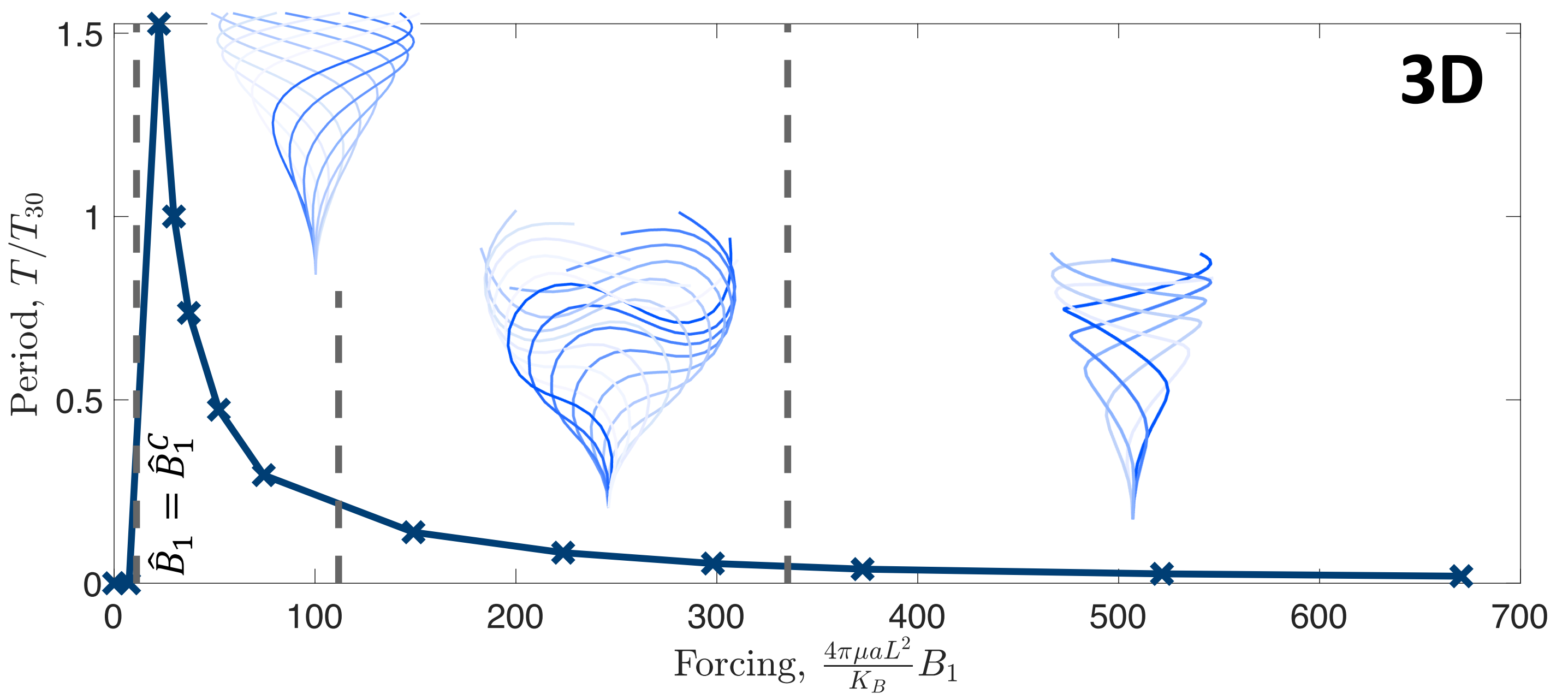


Figure 6: *The period of a filament under a variety of forcings, $\hat{B}_1$. For increased forcing we observe decreasing period and the nontrivial behaviours shown.*

4. RESULTS – TWO FILAMENTS

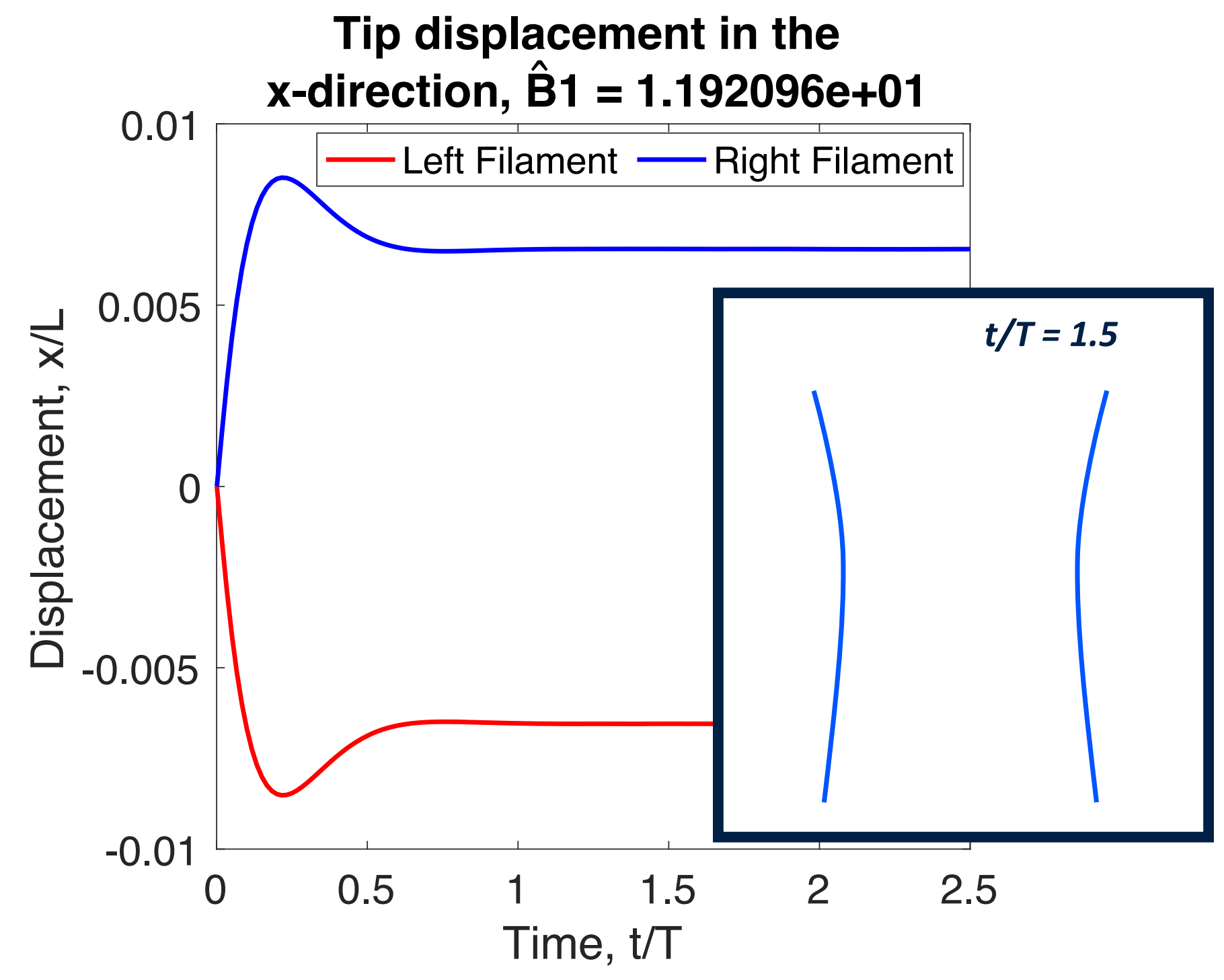
- We also ran simulations for two filaments in 2D. We observe the same bifurcation from a stationary state to sustained oscillations at $\hat{B}_1 = \hat{B}_1^C$ that we found for one filament in 2D/3D:

REGION 1: $\hat{B}_1 < \hat{B}_1^C$
Concave Stationary State

$\hat{B}_1^C$

REGION 2: $\hat{B}_1 > \hat{B}_1^C$
Synchronous Beating

$\hat{B}_1$



REGION 1: $\hat{B}_1 < \hat{B}_1^C$

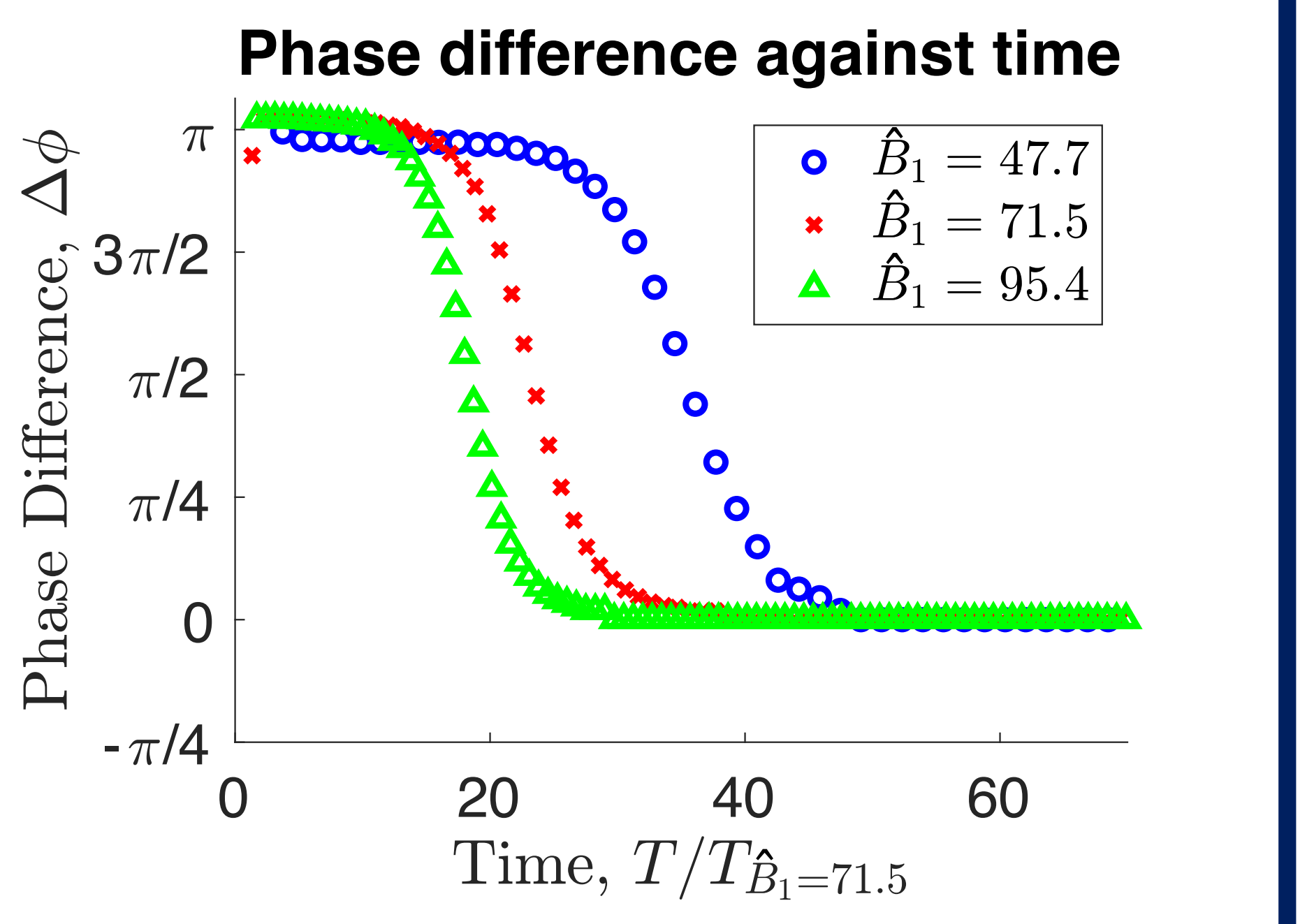
- For small values of the forcing parameter, we observe a concave steady state (see **Figure 7**).
- Here the filaments are closest at their centers, and bend away from each other at the tip.

Figure 7 (left): *The tip displacement over time in the concave regime, and a sketch of the corresponding steady state.*

REGION 2: $\hat{B}_1 > \hat{B}_1^C$

- Filaments synchronize their beat after a transient anti-phase region. Synchronization time decreases with increasing $\hat{B}_1$ (see **Figures 8/9**).
- We note that [1] sees an *anti-phase* beating regime in their model, which we only detect as a transient feature of our simulations.

Figure 8 (right): *The phase-difference over time for three values of the forcing parameter, $\hat{B}_1 > B_1^C$.*



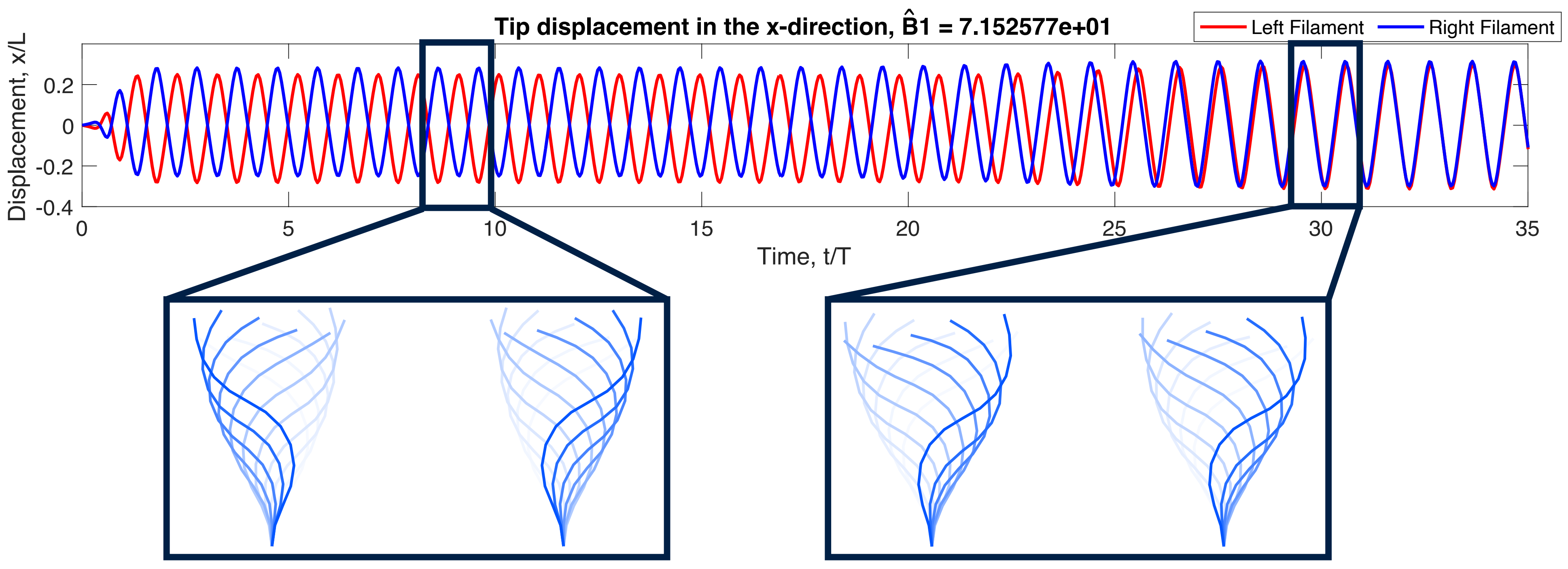


Figure 9 (above): *A tip displacement diagram for a particular value of $\hat{B}_1 > \hat{B}_1^C$, and time-lapsed snapshots of the highlighted regions. We see that the synchronous state is reached after a transient anti-phase region.*

REFERENCES

[1] Dartmouth electron Microscope Facility, Dartmouth College, https://www.dartmouth.edu/emlab/
[2] D. B. Stein et al, 'Swirling Instability of the Microtubule Cytoskeleton', *Physical Review Letters*, 2021
[3] A. Laskar and R. Adhikari, 'Filament actuation by an active colloid at low Reynolds number', *New J Phys*, 2017
[4] S. F. Schoeller, A. K. Townsend, T. A Westwood and E. E. Keaveny, 'Methods for suspensions of passive and active filaments', *Journal of Computational Physics*, 2021

CONCLUSIONS/FURTHER WORK

- Our model uncovers a range of behaviours for both 2D and 3D filament simulations in low Reynolds number flow. Our 2D/1-filament behaviour verifies [2], 3D/1-filament behaviour verifies [3] and 2D/2-filament results compare with [2].
- In future work, we plan to use a more complex surface condition (which contributes a stresslet term) to increase the hydrodynamics in the system and see if we observe the anti-phase regime found in [2] for the 2D/2-filaments case.
- It would also be interesting to investigate the 3D/2-filament scenario, and look at behaviours for more than 2 filaments.