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in Low-Reynolds-Number Medium

Rotem S. Berman

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Swimming and Alignment

in Low-Reynolds-Number Medium

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To Lihu,

My partner at all times.

To Yahel and Peleg,

My gifts.

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List of symbols and abbreviations

General:

μ	viscosity	
р	Pressure	
Re	Reynolds number	
ρ	Density	
In chapter 2:		
ATP	Adenosine tri phosphate	
а	Characteristic radius	
ϵ	Slenderness parameter	
F _n	Force exerted on a stick number <i>n</i> by the fluid	
GC	Geometrical center	
1	Length	
MT	Microtubule	
μт	Micrometer	
N	Number of sticks	
Т	Torque	
Р	The distance of a molecular motor from the center of a stick carried by the motor	
\mathbf{R}_n	Location of the center point of a stick in the lab frame	
θ_{1}	The angle of stick 1 from the x axis in the lab frame	

θ_{2}	The angle of stick 2 from the x axis in the lab frame
U	Speed of the molecular motor advancement on a stick
\mathbf{V}_n	Velocity of the point of the geometrical center of a stick number n
ω_n	Angular velocity around the geometrical center of a stick number n
χ	The distance of a molecular motor from the center of a stick the motor advancing on
In chapter	<u>3:</u>
а	Swimmer's radius
b	Amplitude
с	wave speed, ω/k
C. elegans	s Caenorhabditis elegans
δ	Swimming efficiency
d	Distance between spheres
D	Distance per stroke
ϵ	Slenderness parameter
f_{\parallel}	Longitudinal viscous force proportionality factor
f_{\perp}	Normal viscous force proportionality factor
GC	Geometrical center
К	Local curvature
k	Wave number
N_p	Number of particles in the particle-based swimmer
l	Length of the swimmer

is

\mathcal{L} Expansion order The number of waves a swimmer occupies р Р Rate-of-work expanded in propulsion of an undulating filament RFT **Resistive Force Theory** Т Torque Т Period time of the swimmer's stroke U Rigid body translation velocity of the swimmer Ω Angular frequency of the swimmer's deformation function Rigid body rotation velocity of the swimmer ω W The total work in a single stroke ξ Force ratio

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Abstract

The field of Low-Reynolds-number hydrodynamics describes the realm where viscous forces are dominant over inertial forces, relevant to small objects or objects moving through liquids of high viscosity. This work presents mathematical modeling of two problems from fields governed by low Reynolds hydrodynamics, which are the motion of macromolecules inside biological cells and the swimming of microorganisms.

Inspired by the experimental problem of microtubules arrangement arising from molecular motors connections, we solved the problem of flow-driven re-orientation of connected sticks moving in low Reynolds number medium. The molecular motors were modeled by moving connection points and two connection possibilities were considered. Contrary to former works, we showed that in our modeling, the interaction of a motor which advances on two sticks is highly symmetrical and does not lead to sticks arrangement. However, we found that the alignment of sticks can arise from an interaction which was not considered before, of one motor advancing on one stick and carrying the other. In order to induce alignment, the required properties of the motor are random detachment and a velocity which depends on the angle between the sticks or the sign of the angle change. Going to more complex assemblages, we show that in a non-isosceles triangle of sticks, the angle change diverges when the triangle is closing, causing the system to fall apart. Lastly, the problem of regular polygons made of connected sticks was solved, showing formation of a star assemblage typically observed in the self-organization of microtubules.

The second part of this thesis is devoted to swimming of short undulating filaments, motivated by the propulsion of *C. elegans*. We calculated the distance per stroke and efficiency for a sinusoidal swimmer with wide range of wave numbers and amplitudes, employing particle-based algorithm and resistive force theory (RFT). The comparison between the approaches revealed the limit of the RFT applicability, above which inter-filament hydrodynamic interactions become important and the RFT overestimates the advancement of the swimmer and its swimming efficiency. It was found that for the finite sinusoidal swimmer, there are global maxima of distance per stroke and swimming efficiency. Contrary to the infinite swimmer, the efficiency maximum is located at relatively low values of wave number. The parameters of

biological swimmers were compared with the best sine wave gaits, and most of the swimmers proved to be in the range of parameters appropriate for maximizing the efficiency of swimming, but also showing relatively high distance covered per stroke. Concentrating on *C. elegans*, we calculated its propulsion from the experimental deformation function using the particle-based algorithm, and reached a good agreement with the experimental results. Using this calculation, we were able to compute the propulsion efficiency of the nematode. Compared to the sine wave, both the distance per stroke and the swimming efficiency of *C. elegans* proved to be much higher, demonstrating the importance of geometric optimization of the spatial beating stroke.

1 <u>Outline</u>

This work discusses two different phenomena from the field of low Reynolds hydrodynamics, which describes the realm where viscous forces are dominant over inertial forces, and is relevant to small objects or objects moving through liquids of high viscosity. The first subject, discussed in chapter 2, is the flow-driven re-orientation of sticks connected by molecular motors, which is relevant to the self-organization of microtubules inside the cell. The second part, presented chapter 3, is devoted to swimming of short undulating filaments, motivated by the propulsion of *C. elegans*. In the next section we briefly present the definition of Reynolds number and Stokes equations. The more specific mathematical and biological background for each subject is presented in the relevant chapter, as well as the summary.

1.1 Stokes equations

Navier-Stokes equations for incompressible Newtonian fluid with density ρ and viscosity μ are presented in equation (1.1). **u** is the flow field and p the pressure in the surrounding fluid. The left part includes the inertia contributions, and the right part includes the viscous and pressure forces.

(1.1)
$$\rho\left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right)_{\substack{\text{convective}\\ \text{unsteady}\\ \text{acceleration}}} \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u} \quad , \quad \nabla \cdot \mathbf{u} = 0$$

Transforming to non-dimensional variables according to (1.2), where U is a typical velocity around a body of size L we obtain:

(1.2)
$$\mathbf{u}' \equiv \mathbf{u}/U$$
$$\mathbf{x}' \equiv \mathbf{x}/L$$
$$t' \equiv Ut/L$$
$$p' \equiv pL/\mu U$$
$$Re \cdot \left(\frac{\partial \mathbf{u}'}{\partial t} + \mathbf{u}' \cdot \nabla' \mathbf{u}'\right) = -\nabla' p' + \nabla'^2 \mathbf{u}'$$

where Re stands for the non-dimensional Reynolds number measuring the relative importance of the inertial to viscous forces:

(1.3)
$$Re = \frac{\text{inertial force/unit vol.}}{\text{viscous force/unit vol.}} = \frac{\rho U^2/L}{\mu U/L^2} = \frac{\rho UL}{\mu}$$

We encounter Low Reynolds hydrodynamics when dealing, for example, with the swimming of microorganisms. Typical Re are 10^{-5} for the swimming of *E. coli*, and ~1 for the swimming of the nematode *C. elegans* (both in water). This work discusses the motion of macromolecules and the swimming of small filaments, and thus, is in the realm of both low velocities and small scale. The typical Re we will be dealing with is in the range between 10^{-2} for the first part corresponding to the motion of sticks connected by molecular motor, and Re~1 for the second part dealing with swimming of microorganisms such as nematodes¹.

Small values of Re allow us to neglect the left part of the Navier-Stokes equation (1.2), leading to Stokes equations (1.4)

(1.4)
$$\frac{1}{u}\nabla p = \nabla^2 \mathbf{u} \quad , \quad \nabla \cdot \mathbf{u} = 0$$

Stokes equations are linear and time independent, properties with important consequences to the swimming in such medium, as discussed in section 3.1.1. Several solution methods have been developed for cases which are too complicated to solve analytically. Among them the Resistance Force Theory (RFT) method for slender filaments, and the more accurate slender body theory. To calculate the swimming of short filaments we'll be using the RFT method relevant to locally slender bodies (sections 0, 3.2.3), and numerical algorithm of the solution of flow around chains of spheres (sections 3.1.3, 03.2.2). The problem of connected sticks is more simple, since the sticks has very high aspect ratio, thus can be solved using the slender body approximation detailed in section 2.1.5.

¹ The question whether indeed low Re is applicable to the nematode swimming is addressed specifically in 0.

2 Sticks in Honey: Motion of sticks connected by molecular motors

In this chapter we discuss the flow-driven re-orientation of sticks connected by molecular motors, moving in low Reynolds number medium. The problem was motivated by the phenomenon of self-organization of microtubules inside the cell, called cytoplasmic streaming. Section 2.1 describes this phenomenon and the biological components which take part in it. We detail the properties of the biological components, which dictate the properties of our simulated sticks and motors. Afterwards, we survey former theoretical works which dealt with similar problems. Section 2.2 presents our derivations and simulations, which employed a different modeling of the motors' connections than considered before, allowing significant influence of the hydrodynamic force on the motion of the sticks. This section also presents the main results of the chapter, namely, the analysis of the interactions between two connected sticks, with two possible connection types considered. Next, we continue to larger assemblages providing nice examples of combined influence of geometry and hydrodynamic forces on sticks organization. These include three connected sticks which form a dynamic triangle, and then *N* sticks connected to form regular polygon transforming into a star shape. Section 2.3 summarizes this part of the work.

2.1 Background

2.1.1 Self-organization of MT in drosophila egg

During the development of Drosophila oocyte, a dramatic self-organization phenomenon occurs, which is called "cytoplasmic streaming"². In this process, the array of microtubules in the cell transforms from a random network into an aligned formation of spirals, followed by vigorous mixing of the cell content by organized vortices which span the whole cell cytoplasm, as shown in Figure 1. A similar self-organization process has been produced in in-vitro systems much simpler than the oocyte, comprising of microtubules (MTs) and artificially created complexes of molecular motors. In both systems, there are open questions concerning the nature

²The term "cytoplasmic streaming" is used also for normal inner cell transport, and for streaming inside plant cells which has different characteristics.

of the molecular interactions which create the forces aligning the MTs. Most importantly, the role of the hydrodynamic interactions between the MTs and their surrounding medium has not been fully investigated.

The hydrodynamic drag force acting on bodies inside the cell ($\sim 10^{-15}$ N) is much smaller than the measured stall force of molecular motors ($\sim 10^{-12}$ N), and therefore it is usually neglected when problems of molecular motors dynamics are considered. However, in crowded solutions where the effective viscosity can reach 1000 times that of water [1], the hydrodynamic interaction becomes comparable to the force exerted by molecular motors. Also, the hydrodynamic interactions were found to change the motion of motors in ordered arrays of biofilaments [2], and are therefore an important force in the organization of the system. We'll show that for sticks connected by simple moving connection points which represent the motors, the hydrodynamic drag is a sufficient force which causes organization of the system is several cases.



Figure 1: Slow verses fast cytoplasmic streaming in drosophila oocyte. the visualization was done by merging ten successive images taken at 7 seconds intervals. The green channel visualizes autofluorescent yolk granules and GFP, and the red particles represent unidentified organelles that reflect 568 nm light. (I) In a wild-type oocyte at stage 9, slow seething is observed. (J) stage 9 oocyte that was treated to display premature fast streaming. The streaming causes the particles to appear as lines in the merged image, showing the created vortex. The picture was taken from [3].

2.1.2 **Biological components**

In this section we describe shortly the basic components included in the experiments and systems which were simulated. Most of the material in this section was summarized from [4].

Microtubules

Microtubules (MTs) are long protein polymers. Their function in the cell is mainly as tracks for the advancement of molecular motors (see below). They have the structure of a hollow cylinder with an outer diameter of 25 nanometer, and their typical length inside the cell is in the order of microns, making their aspect ratio very high (\sim 100). Moreover, they have high rigidity - their persistence length³ is 6 millimeters, meaning that they can be regarded as rigid rods for many purposes. MTs are polar structures; their two edges are marked as "the plus end" where fast polymerization and depolymerization occurs and "the minus end" which changes much slower. Molecular motors advance on MTs in one direction (either from + to -, or vice versa), which depends upon the motor kind.

MTs display dynamic instability: individual MT switch randomly from growth to fast depolymerization (called a "catastrophe"). The switching time between states is in the order of minutes, and the polymerization/depolymerization rates are 1 μ m/min. and 10 μ m/min, respectively.

The dynamic instability was described empirically [5] by a model with four parameters: the growth rate, the shrinkage rate, and the frequencies of transitions between the states. These frequencies vary between 0.01sec^{-1} for a catastrophe (growth to shrinkage), and 0.02sec^{-1} for rescue (shrinkage to growth). Since the probability of a transition from growth to shrinkage is about half the probability of the change from shrinkage to growth, in a steady population the distribution of the MTs is that 2/3 of them are growing and 1/3 shrinking.

³The persistence length of a polymer can be defined as the decay length of the tangent-tangent correlation function.

For the purpose of this work, the MTs were modeled as rigid rods with high aspect ratio. The MTs' length change during the motors advancement can be calculated as follows: for a typical motor advancing at 1 μ m/s on an average MT of length 5 μ m, the probability of a transition from growth to shrinkage would be⁴ 10%, and from shrinkage to growth 5%. The maximum length change during motor advancement would be 16% shortening or 1.6% growth.

The influence of the length change on the interaction between sticks is presented at the end of section 2.2.2.1, and shown to be negligible. Therefore, in the calculation of the motion of pairs and assemblages of connected sticks, we will ignore the length change of the MTs during the motors advancement and regard them as constant length sticks.

<u>Kinesin</u>

Molecular motors are complex proteins which convert chemical energy in the form of ATP into mechanical work. We focus on conventional kinesin (kinesin 1), a motor that advances on microtubules. Kinesin mediates inner cell transport by binding to vesicles and organelles and carrying them, using the MTs as a track. Kinesin has two heads which bind interchangeably to the microtubule, and a tail which binds to the designated cargo, e.g., a vesicle in the cell or a bead in the in-vitro experiments. The dimensions of kinesin are 7x4.5x4.5 nm, and its step size is 8 nm. It is a processive motor, meaning that a single motor moves continuously on the surface of a MT for a few μ m corresponding to hundreds of steps, with a constant probability of detachment of 1% per step [6]. The velocity ranges from 0.5 to 2 μ m/s depending on conditions, and the stall force is ~ 6 pN, as measured by optical tweezers [4].

Kinesin is considered to be a non-cooperative motor, meaning that it binds alone to a vesicle. Interaction between two MTs can occur also by the binding of one kinesin to two MTs, a possibility indicated by a few observations ([7] and references therein).

The rotational freedom of kinesin attached to a cargo was examined in relatively few experimental works, with contradicting conclusions. In [8], the torsional flexibility of kinesin was found to be very low, allowing the binding of cargo in any direction. However, in [9], no

⁴ Assuming a Markov process with constant probability of 0.02 per second, and 5 tries, the probability of at least one direction change would be $1-(0.98)^5 = 10\%$

rotations of MTs connected to kinesin motors were found. Since the advancement mechanism of kinesin deduced from [9] was later shown to be wrong, we will base our model on the most recent work we found [10]. The work examined the rotational diffusion of beads connected to kinesin and concluded that the stem of the kinesin motor acts as a swivel and that rotational freedom during cargo transport can be significant.

In the next section (02.2), we will model the interaction arising from the binding of one and two motors to two MTs. The motors will be modeled by moving connection points, acting as free swivels for MTs rotation.



Figure 2: Engineered kinesin complexes advancing on microtubules. This schematic representation shows four kinesin motors joined together by streptavidin. This complex advances on the MTs in the plus end direction and creates force that will pull the plus ends to each other. The picture was taken from [12].

2.1.3 In vitro experiments

The formation of patterns by systems of MTs and molecular motors has been demonstrated in in-vitro experiments containing very few ingredients. In a system containing only kinesin, ATP, and fixed length MTs, rapid formation of asters⁵ of MTs were observed [11].

Nedelec et al. [12] made use of engineered kinesin complexes, in which two motors or more were connected by a biotin - streptavidin link (see Figure 2). With fixed length MTs, they repeated the asters formation found in [11]. In addition, they observed the formation of a stable MTs vortex in a system of polymerizing and depolymerizing MTs and motor complexes. At first, the MTs organized into an aster, which transformed to a vortex when the MTs continued to grow (see Figure 3). The formation of the vortex took ~3 minutes from the initiation of the MTs polymerization, and its diameter was ~90 μ m. In larger containers, a variety of patterns were observed, depending on the concentration of motors (see Figure 4).



Figure 3: The formation of a vortex in a system of microtubules and kinesin. Left - after ~0.5min from the polymerization start, uniform solution of microtubules. Middle - after ~1.5min, formation of an aster in the center of the chamber. Right - after ~3min, a steady state vortex is formed. Adapted from [12].

⁵An aster is a structure of MTs in the form of a star, with the MTs radiating from the center outward



Figure 4: The system of microtubules and motors complexes organizes to different large scale patterns depending on the motors concentration. d. In a low concentration of motors $<15\mu g/ml$, a lattice of vortices is formed. a. At a slightly higher concentration $\sim 25\mu g/ml$ a lattice of asters and vortices is formed. b. An irregular lattice of asters is obtained when raising the concentration more $\sim 37.5\mu g/ml$. c. Bundles of microtubules created at high motor concentration $\sim 50\mu g/ml$. The picture was taken from [12].

In low concentration of motors, the MTs organized into a lattice of vortices (Figure 4d). In higher concentrations, the pattern shifted gradually to a lattice of asters (Figure 4a,b), and finally became an irregular MTs bundle (Figure 4c), in a very high concentration of motors. The systems were quasi two dimensional, as the experiments were done in chambers 5 μm deep, forcing the MTs to be nearly parallel to the plane of the sample.

In a following work, the same group [13] studied systems with two kinds of motor complexes, kinesin and NCD (motors which advance on MTs in the opposite direction, compared to kinesin). They observed combinations of asters and vortices, depending on the relative concentration of the two kinds of motors.

2.1.4 Theoretical models

Various theoretical approaches were proposed to reproduce the macroscopic pattern observed in the in-vitro experiments described above [12-21].

In [12] and [13] numerical simulations were done, which succeeded in reproducing the experimental patterns. This approach was later extended to the creation of a detailed computer program ("cytosim") [22] for the calculation of cytoskeleton dynamics. Lee and Kardar [17] arrived to two coupled nonlinear PDEs for the local motor number and the local MTs orientation field. The motors action was modeled by coupling of neighboring tubule orientation. In [16] differential equations for general active polar gels were written. The equations were based on conservation laws and derived using the approach of non-equilibrium thermodynamics. The interaction between filaments, induced by the motors, was modeled as an addition to the viscoelastic properties of the medium. Liverpool and Marchetti [18] derived equations for the filament probability distribution function and introduced the local velocity created by the microscopic motors interaction. They included the fluid resistance by using anisotropic friction coefficients for the filaments. Aranson and Tsimring [21] obtained equations for the probability distribution of the orientation angles of the filaments. The motors interaction was simulated as a collision between two filaments which changes their relative angle. The angle change was calculated from balance of torques and forces due to the motor motion, but the anisotropy of the translation friction was neglected.

The microscopic alignment of stiff rods connected by motors was explored in [23]. The motors were represented by springs, and the fluid resistance was taken into account by a rotational friction coefficient. The following motors characteristics were considered: a linear force-velocity relation, the attachment-detachment kinetics and random fluctuations in the motor's force. In a following work [24], the case of semi-dilute mixture of motors and rods was considered, by inclusion of the interaction of multiple connected rods in a Brownian dynamic type simulation. The effect of noise on the pattern formation robustness was investigated. The emergence of bundles and vortices was shown in both the dilute and semi-dilute cases. The semi-dilute case showed more robustness of the organization pattern to additive thermal noise. Surprisingly, the introduction of multiplicative noise originating from the motors' fluctuations

increased the organization process and contributed to faster formation and coalescence of vortices.

Similarly to [23], we investigated the alignment of pairs of sticks due to the action of molecular motors. In our model, the motors are represented by rigid constraints instead of springs. A significant difference is that we take into consideration the possibility of free rotation of the sticks around the interaction point. This is a more suitable modeling of the connection point (see discussion on section 2.1.2) than the assumption of springs used before. The free rotation changes the nature of the main interaction contributing to the sticks arrangement in [23,24], which is the interaction of two sticks connected by two motors. We show that in our model, this interaction does not contribute to the sticks alignment. We consider a different interaction, which is the connection of a single motor with two sticks, and show that it can decrease the angle between the sticks and thus lead to alignment. We also investigate the case of three connected sticks and the interaction of N sticks in a regular polygon.

2.1.5 <u>Resistance matrix for a slender body</u>

For a rigid particle we will use the non-slip condition - $\mathbf{u} = \mathbf{U}_o + \boldsymbol{\omega} \times \mathbf{r}_o$, where O is any point on the particle, \mathbf{U}_o is the velocity of the point and $\boldsymbol{\omega}$ is the angular velocity of the particle.

Due to the linearity of the Stokes equations (1.4), the relations between the forces and velocities are linear, hence the force and torque can be written as [25]:

$$\mathbf{F} = -\mu \mathbf{K} \cdot \mathbf{U}_o - \mu \mathbf{C}_o^{\mathrm{T}} \cdot \boldsymbol{\omega}$$

 $\mathbf{T} = -\mu \mathbf{C}_o \cdot \mathbf{U}_o - \mu \mathbf{\Omega}_o \cdot \boldsymbol{\omega}$

where \mathbf{K} , $\mathbf{\Omega}_o$ and \mathbf{C}_o , are second rank tensors which are intrinsic geometrical properties of the body. $\mathbf{C}_o^{\mathrm{T}}$ is \mathbf{C}_o transposed. \mathbf{K} is the translation tensor, it is symmetric and does not depend on the origin point. $\mathbf{\Omega}_o$ is the rotation tensor, it is also symmetric but depends on the location of the origin O. \mathbf{C}_o is the coupling tensor, it depends on the location of O and represents the coupling between the translational and rotational motions. It is not generally symmetric. When transforming from a point O on the body to another point P, the following transformations apply:

$$\mathbf{U}_p = \mathbf{U}_o - \mathbf{r}_{op} \times \boldsymbol{\omega}$$

- $\mathbf{C}_p = \mathbf{C}_o \mathbf{r}_{op} \times \mathbf{K}$
- $\boldsymbol{\Omega}_{p} = \boldsymbol{\Omega}_{o} \mathbf{r}_{op} \times \mathbf{K} \times \mathbf{r}_{op} + \mathbf{C}_{o} \times \mathbf{r}_{op} \mathbf{r}_{op} \times \mathbf{C}_{o}^{\dagger}$

Where \mathbf{r}_{op} is the vector connecting point O to point P on the body.

For two dimensional (plane) motion we can define a resistance matrix M, which defines the relations between the force and torque to the linear and angular velocities:

(2.1)
$$\begin{pmatrix} F_x \\ F_y \\ T \end{pmatrix} = \mathbf{M} \begin{pmatrix} \mathbf{v}_x \\ \mathbf{v}_y \\ \mathbf{\omega} \end{pmatrix}, \ \mathbf{M} = \begin{pmatrix} K_{11} & K_{12} & C_{31}^* \\ K_{12} & K_{22} & C_{32}^* \\ C_{31} & C_{32} & \Omega_{33} \end{pmatrix}$$

When * signifies the complex conjugate. A slender body is defined as a body that its characteristic diameter 2a, a being the characteristic radius, is much smaller than its length l, so that $\epsilon = \frac{2a}{l} \ll 1$. ϵ is called the slenderness parameter. It is possible to solve the Stokes' equations for a flow around such a body as an asymptotic approximation in ϵ . This was done by Batchelor [26] for bodies of revolution, and by Cox [27] for a straight or slightly curved slender body with circular cross section. For such bodies, it was found that the resistance to motion in the direction perpendicular to their axis is twice the resistance to motion in the direction parallel to their axis:

$$F_{\perp} = 8 \frac{\pi \mu l}{\log\left[\frac{2}{\epsilon}\right]} U_{\perp}$$

$$F_{\parallel} = 4 \frac{\pi \mu l}{\log\left[\frac{2}{\epsilon}\right]} U_{\parallel}$$

The problem of sticks connected by molecular motors is motivated by the flow around microtubules, which are very slender ($\frac{2a}{l} < 0.001$), have a circular cross section and very low curvature. These properties justify the use of the slender body approximation for the solution of the problem.

2.2 Results: Sticks in viscous fluid

2.2.1 Motion of a single stick pulled in constant speed

First we present the solution for the simplest case of a stick carried by a molecular motor, assuming that the motor is a moving connection point carrying the stick in the direction of the X axis, as presented in Figure 5. A stick with length *l* is pulled in constant speed V in a fluid having viscosity μ . As explained in section 2.1.5, we apply the slender body approximation to write the resistance matrix for the stick's plane motion. In the stick's body-frame the relations are:

(2.2)
$$\begin{pmatrix} F_x \\ F_y \\ T \end{pmatrix} = \frac{4\pi\mu}{\log\left[\frac{2}{\epsilon}\right]} \begin{pmatrix} l & 0 & 0 \\ 0 & 2l & 0 \\ 0 & 0 & \frac{l^3}{6} \end{pmatrix} \begin{pmatrix} V_x \\ V_y \\ \omega \end{pmatrix}$$

Using the following notation:
$$\mathbf{F} = \begin{pmatrix} F_x \\ F_y \\ T \end{pmatrix}$$
, $k = \frac{4\pi\mu}{\log\left[\frac{2}{\epsilon}\right]}$, $\mathbf{M}_{body} = \begin{pmatrix} l & 0 & 0 \\ 0 & 2l & 0 \\ 0 & 0 & \frac{l^3}{6} \end{pmatrix}$, $\mathbf{V} = \begin{pmatrix} V_x \\ V_y \\ \omega \end{pmatrix}$,

we can write the relations in the lab frame as :

(2.3)
$$\mathbf{F} = k\mathbf{M}_{lab}\mathbf{V}$$
$$\mathbf{M}_{lab} = \mathbf{R}\mathbf{M}_{body}\mathbf{R}^{-1}$$

Where **R** is the rotation matrix at angle θ around the Z axis, θ being the angle of the stick from the X axis. \mathbf{M}_{body} is the mobility matrix of the stick in its body frame, and \mathbf{M}_{lab} is its mobility matrix in the lab frame.



Figure 5: A single stick pulled in the x direction by a molecular motor. GC is the location of the geometrical center, q is the connection point of the molecular motor, pulling the stick at velocity V_q in the x direction. χ is the vector from the geometrical center to the motor connection point.

We define χ as a vector from the geometrical center of the stick to the point q of the velocity activation, $\chi = \chi (\cos \theta, \sin \theta)$, $\frac{-l}{2} \le \chi \le \frac{l}{2}$. Then, the velocity of the point q of the stick is

$$\mathbf{V}_{q} = \mathbf{V}_{GC} + \boldsymbol{\omega} \times \boldsymbol{\chi}$$

 $V_{\rm GC}$ is the velocity of the geometrical center of the stick, and ω its angular velocity. The torque on the stick is:

$$(2.5) T = \chi \times F$$

If a stick is pulled at point q at a velocity V_q , then from equations (2.4),(2.5),

(2.6)
$$V_{GCx} = V_{qx} + \omega \chi \sin \theta$$
$$V_{GCy} = V_{qy} - \omega \chi \cos \theta$$
$$T_z = -\chi \left(F_x \sin \theta - F_y \cos \theta \right)$$

τ7

Where $\omega = (\omega)_z$. Inserting these into equation (2.3) we arrive to equations for the forces as a function of θ and the angular velocity as a function of θ , $\omega = f(\theta)$. From the latter we solve for $\theta(t)$ and calculate the forces.

For example we present the results for a stick of length l=1, starting aligned with the y axis and pulled from its end point in velocity V=1 at the x direction. The stick advances in the x direction while rotating, until it aligns with the velocity direction. In this case $\theta(t) = 2\operatorname{arccot}(e^{3t/2})$, which is shown in Figure 6a. Figure 6b displays the velocity of the geometric center of the stick, and Figure 6c depicts the forces as a function of time.



Figure 6: (a) The angle as a function of time, for one stick pulled at the x direction, $\theta(t) = 2 \operatorname{arccot} \left(e^{3t/2} \right)$. (b) The x and y velocities of the geometric center of the stick as a function of time. (c) The forces on the stick's GC as a function of time.

2.2.2 Two sticks

Now we turn to the more complicated problem of the motion of two connected sticks. We considered two connection types which dictate the relative velocity of the sticks. Apart from the different kinematic constraints, the equations in both cases are similar. The first possibility considered, displayed in the following section, is one motor which advances on one of the sticks and carries the other. We show the function $\theta_{difference_final}(\theta_{difference_initial})$ originating from this interaction and demonstrate how it changes with different possible motor properties. Afterwards, (section 02.2.2.2) we present the interaction emerging from two connected motors advancing on two sticks, showing that in this case, the interaction is highly symmetrical and does not contribute to the sticks' alignment.

2.2.2.1 Motor advancing on one stick and carrying the other

A motor connected to point P on stick 1 with length l_1 , advances in velocity u on stick 2 with length l_2 . The parameters are:

	P - the distance of the motor from the center of stick 1.
(2,7)	χ - the distance of the motor from the center of stick 2.
(2.7)	θ_1 - the angle of stick1 from the x axis in the lab frame.
	θ_{1} - the angle of stick 2 from the x axis in the lab frame.

The geometry is shown in Figure 7. We use the notation:

(2.8)
$$\mathbf{P} = P[\cos(\theta_1), \sin(\theta_1)]$$
$$\chi = \chi[\cos(\theta_2), \sin(\theta_2)]$$

Notice that P does not vary in time, $-\frac{1}{2}l_1 \le P \le \frac{1}{2}l_1$. χ varies in time as the motor advances, according to $\chi(t) = \chi_0 + ut$. $-\frac{1}{2}l_2 \le \chi(t) \le \frac{1}{2}l_2$ and this gives the time of the motor detachment at the end of stick 2.


Figure 7: A motor connected to stick 1 advances on stick2. The motor point is marked in red. P is the distance of the motor from the geometrical center of stick 1, χ is the distance of the motor from the geometrical center of stick 2.

Equations of motion:

We write equations (2.3) for each stick requiring force- and torque-free motion:

(2.9)
$$\sum \mathbf{F} = 0$$
$$\sum T_z = 0$$

The forces and torques can be written explicitly as $F_{x1} = F_x$, $F_{y1} = F_y$, $F_{x2} = -F_x$, $F_{y1} = -F_y$, $\mathbf{T}_1 = \mathbf{P} \times \mathbf{F}$, $\mathbf{T}_2 = -\chi \times \mathbf{F}$. The motor enforces the kinematic constraint for the point of motor connection, which moves on both sticks with the same velocity:

(2.10)
$$\mathbf{V}_{gc1} + \boldsymbol{\omega}_1 \times \mathbf{P} = \mathbf{V}_{gc2} + \boldsymbol{\omega}_2 \times \boldsymbol{\chi} + u [\cos \theta_2, \sin \theta_2]$$

We solve the system of equations (2.3), (2.9),(2.10), to obtain $\theta_1(t)$, $\theta_2(t)$, with the parameters *P*, χ and the initial angles.

Sticks of different lengths: When $l_1 < l_2$, the drag on stick 2 will be higher than the drag on stick 1, and stick 2 will function as an "anchor". The interaction will be similar to the case of one stick pulled by a motor, (section 2.2.2.1), and will result in the anti-aligning of stick 1 with stick 2 (corresponding to an angle of π). When $l_2 < l_1$, the interaction time *t* will be very short, so the final angle tends to the initial angle. Figure 8 depicts the final angle of stick 1 as a function of the length ratio between the sticks, l_1/l_2 , for two sticks connected at their starting point $(P = -1/2l_1, \chi = -1/2l_2)$, and starting angles of $\theta_{1i} = \pi/6$, $\theta_{2i} = 0$.



Figure 8: The final angle between the sticks as a function of the length ratio, l1/l2, for two sticks connected at their starting point $(P = -1/2l_1, \chi = -1/2l_2)$, and starting angles of $\theta_{di} = \pi/6$.

Sticks with the same length l = l = 1: Figure 9 shows the final angle between the sticks as a function of the initial angle for the parameters $P = \pm 1/2$, $\chi = -1/2$. The function θ_{df} can be fitted to an analytical function H Shown in fine lines in Figure 9.

(2.11)

$$H(\theta_{di}, P, \chi) = \theta_{di} + \tanh\left(-4P \cdot f_{\chi}\right) \sin\left(\theta_{di}\right) + \left(2.5\left(P \cdot f_{\chi}\right)^{2} - 7\left(P \cdot f_{\chi}\right)^{4}\right) \sin\left(2\theta_{di}\right) + f_{\chi} = 0.52\chi^{2} - 0.91\chi + 0.35$$



Figure 9: The final angle between the sticks as a function of the initial angle, for equal length sticks with the parameters $P = \pm 1/2$, $\chi = -1/2$. The analytical function H fitted to the results is shown in fine lines.

Solving $\theta_{diff}(t)$ for many initial parameters we can map the function $\theta_{df}[\theta_{di}, P, \chi]$. (From here we mark the final angle between sticks as θ_{df} and the initial angle between the sticks as θ_{di}). In Figure 10a and Figure 10b the function is plotted for different values of P and χ . It can be seen that for a fixed value of χ , different P values control the curvature of the function, and $\theta_{df}[\theta_{di}, P = 0, \chi] = \theta_{di}$. In addition the functions have the symmetry property of

$$\theta_{df}\left[\theta_{di}, \boldsymbol{P}, \boldsymbol{\chi}\right] = \theta_{df}^{-1}\left[\theta_{di}, -\boldsymbol{P}, \boldsymbol{\chi}\right]$$

From Figure 10b we see that for a fixed value of P, different χ values also control the function curvature, similar to the effect of P, but here the non-interaction case is when $\chi = 1/2$. This is the case of a motor which starts at the end of stick 2 and falls off immediately.



Figure 10: (a) The function $\theta_{df} \left[\theta_{di}, P, \chi \right]$ for $\chi = -1/2$ and different values of $P \cdot P = 0$ is the case of a motor which starts at the middle of stick 1 so the angle does not change during the motor advancement. (b) The function $\theta_{df} \left[\theta_{di}, P, \chi \right]$ for P = -1/2 and different values of $\chi \cdot \chi = 1/2$ is the case of a motor which starts at the end of stick 2 and immediately falls off.

Final angle between the sticks for different motor properties

Looking for possible processes driving arrangement of the sticks, we calculated the final angle between sticks for different motor properties. The experimental data on molecular motors properties when rotated and distorted is scarce, thus we checked various assumptions and searched for properties which will give rise to asymmetry of the functions. Figure 11 displays the final angle of stick 1 as a function of the initial angle for $P = \pm 1/2$, $\chi = -1/2$, which means that the motor is advancing on stick 2 from its start, and connected either to the beginning of stick 1 (P = -1/2) or the end of stick 1 (P = +1/2). A function for which

 $\theta_{df} \left[\theta_{di}, P, \chi \right] \neq \theta_{df}^{-1} \left[\theta_{di}, -P, \chi \right]$ will give rise to drift of the angle in recurring interactions and a possible arrangement of the sticks.

(a) Motor detachment in a constant angle θ_s : one possible assumption is that for a certain angle between the sticks the conformation of the motor becomes too distorted and it has to detach from one of the sticks. The function $\theta_{df}(\theta_{di})$ for detachment at a constant angle $\pi/2$ is shown in Figure 11a. It can be seen that the function is symmetric as was the original function $\theta_{df}[\theta_{di}, P, \chi]$.

(b) Motor with a detachment probability constant in time: A known property of the motors is that they detach from the microtubules with a constant probability [6]. Statistic detachment of the motor from the stick was simulated using a numerical algorithm. Each time step the motor had a probability to detach which is proportional to the time step length. We used 100 time steps to simulate the advancement of a motor with velocity 1 on a stick with length 1. The initial angle as a function of the final angle, for an average of 50 calculations is shown in Figure 11b. As expected, the function is symmetric as was the original function $\theta_{df} [\theta_{di}, P, \chi]$.

(c) Detachment probability constant in time, combined with advancement velocity dependent on the angle: A viable assumption is that the velocity of the motor depends on its conformation. Using that assumption we changed the velocity of the motor as a function of the angle between the sticks. The function chosen was $u(\theta_d) = \frac{0.9}{\pi^2}(\theta_d - \pi)^2 + 0.1$, shown in the inset of Figure 11c. For aligned or anti-aligned sticks the velocity is high, and decreases as the angle between the sticks rises. In this case, the line fit to the function at small angles has the property that $\theta_{df} \left[\theta_{di}, P, \chi \right] < \theta_{df}^{-1} \left[\theta_{di}, -P, \chi \right]$. The initial slope of $\theta_{df} \left[\theta_{di}, 1/2, -1/2 \right]$ is ~ 0.52 , while the initial slope of $\theta_{df} \left[\theta_{di}, -1/2, -1/2 \right]$ is $\sim 1.72 \approx 1/0.58$. This asymmetry can give rise to slow arrangement of the sticks in multiple interactions.

(d) Detachment probability constant in time, combined with advancement velocity dependent on the angle change: along the lines of the former property, it can be assumed that the important parameter affecting the motor velocity is not the value of the angle between the sticks, but rather its change – whether it is closing – thus the motor deforms to a more favorable conformation, allowing faster advancement, or opening and increasing the stress of the motor, thus reducing the motor velocity. Figure 11d shows the results for a motor with such property. When the angle closes, $\frac{\partial \tilde{\theta}}{\partial t} < 0$, and $u_{close} = 1$, and when the angle opens, $\frac{\partial \tilde{\theta}}{\partial t} > 0$, $u_{open} = \frac{1}{2}$, for $\tilde{\theta} = \min(\theta_d, 2\pi - \theta_d)$. Here also, as in property (c), $\theta_{df} [\theta_{di}, P, \chi] < \theta_{df}^{-1} [\theta_{di}, -P, \chi]$. The initial slope of $\theta_{df} [\theta_{di}, 1/2, -1/2]$ is ~ 0.54, while the initial slope of $\theta_{df} [\theta_{di}, -1/2, -1/2]$ is ~1.5 ≈ 1/0.66. This asymmetry makes this property a viable candidate to create alignment of the sticks.



Figure 11: The final angle between sticks as a function of the initial angle for $P = \pm 1/2$, $\chi = -1/2$, for different motor properties. (a) Motor detachment in a constant angle $\theta_s = \pi/2$. (b) Motor with a detachment probability constant in time. (c) Detachment probability constant in time, combined with advancement velocity dependent on the angle difference. The inset shows the velocity of the motor as a function of the angle. (d) Detachment probability constant in time, combined with advancement velocity constant in time, combined with advancement velocity dependent on the angle change. The line of $\theta_f = \theta_i$ is shown in b,c,d, for more clarity.

Arrangement due to multiple interactions

Recent works [21,28] showed that multiple non-elastic collisions between sticks lead to nematic order. To show that, they used fully stochastic simulations which kept track of the location of each stick geometrical center and its motion due to interactions between the other sticks, thermal noise and noise from motors steps.

The interactions suggested above are more accurate than the simplistic collisions used in [21,28], and can be used in a similar simulation to confirm their capability in creating order. A "Zero order" of such a simulation is calculating the angle between two sticks due to multiple interactions between them. To demonstrate how the property of "advancement velocity dependent on the angle change", (option **d** above) leads to nematic order, we calculated the angle between two sticks after multiple interactions, each interaction starting with the final angle of the last encounter, but with random P value (contact point of stick 1 on stick 2). The χ value was taken as $\chi = -1/2$, to allow the motor to walk along the full length of stick 2 or until it detaches randomly. Since the P value determines if the final angle is higher (for P<0) or lower (for P>0) than the initial angle, the emerging behavior resembles one dimensional biased random walk, as can be seen in Figure 12a. Figure 12 demonstrates how this interaction leads to a complete alignment of the sticks. Figure 12a shows a single instance of the multiple interaction alignment, while Figure 12b displays an average of 50 sequences of multiple encounters, each sequence is different due to the random detachment of the motor and the random P value in each encounter. This figure displays how the change in the reduced velocity in opening vs. closing leads to alignment while equal velocities show no arrangement on average.



Figure 12: Multiple interactions between a pair of sticks, with a motor which advances in half the velocity when the angle closes (property d in the text), $\chi = -1/2$ and random P in each interaction. (a) A single instance of the multiple interactions alignment. (b) Average over 50 repetitions of multiple encounters, for $u_{open} = u_{close}$ - in blue, vs. $u_{open} = 0.5u_{close}$ - in green.

Effect of stick's length change

In order to check the influence of the MTs length change (see section 2.1.2), we recalculated the basic interaction for a motor advancing on one stick and carrying the other, while including a shortening of 16% of the carried stick during the motor advancement. Here the motor is simple and do not include any of the properties (a-d) discussed before. We didn't include length change of the stick the motor advances on, since this stick's motion is negligible during the interaction, meaning that its length change can mostly influence the motion of the geometrical center of the system and not the angle between sticks.

Figure 13 displays the function $\theta_{df} [\theta_{di}, P, -1/2]$ for different values of P. The solid lines represent the original function without the stick's shortening, as shown in Figure 10a, while the dashed lines represent the function for a stick with 16% shortening. For clarity, the values of P > 0 are displayed separately.



Figure 13: The function $\theta_{df} \left[\theta_{di}, P, \chi \right]$ for $\chi = -1/2$ and different values of P. The solid lines represent the original function without the stick's shortening, while the dashed lines represent the function for a stick with 16% shortening during the motor's advancement. (a) For values of $P \le 0$; (b) For values of P > 0. (the full line of P = 1/2 is below the full line of P = 0.4).

It can be seen that the length change affects the function in two different ways. One influence is for $P \approx 0$, for which the stick's shortening transforms the interaction from weak anti-aligning or symmetric interaction to weak aligning interaction (compare dashed and full green lines in Figure 13a). The symmetric interaction in this case will occur for P = -0.045 (not shown). A more dominant effect is for P > 1/3. In these interactions, the sticks' disintegration includes the location of the motor, thus ending the interaction in a shorter time than in the constant length case. Thus, for P = 1/2, the stick's shortening prevent the interaction altogether, as can be seen from the purple dashed line in Figure 13b.

From this calculation we can conclude the influence of the length change on the entire sticks population. As discussed before (section 2.1.2), 2/3 of the sticks are growing slowly (growth of 1.6% of the stick's length growth during the motor's advancement). The influence of the growth of the interaction would be a slight change in the symmetry of the function at $P \approx 0$ values. For the 1/3 of the sticks which are shortening, the main influence would be on P > 1/3 values,

where part of the aligning interactions would end in a shorter time. In order to change the time of the interaction, the shortening of stick 1 (the carried stick) needs to outrun the motor's advancement to the end of stick 2. This criterion translates to $\frac{l_1}{u}(\frac{1}{2}-\chi) < \frac{l_2}{u_s}(\frac{1}{2}-P)$, where u_s is the shortening velocity of the carried stick (stick 1). For typical values of $u = 1\frac{\mu}{s}$, $u_s = \frac{1}{6}\frac{\mu}{s}$, (see section 2.1.2), and equal length sticks, a shorter interaction time will occur for $\frac{l_2}{2}$ of the shortening sticks interaction with P > 1/3.

Overall, the length change will reduce the interaction time of 2.5% of the aligning interactions, and will transform 1.5% of the weak anti-aligning interactions into weak aligning interactions. Therefore, the length change of the MTs is expected to have a negligible effect on the global alignment of sticks in multiple interactions.

2.2.2.2 <u>Two motors advancing on two sticks</u>

A second possible interaction between sticks and molecular motors is the case where two connected motors are advancing on two sticks. Each motor is advancing on one of the sticks, and the motors are connected to each other thus enforcing a kinematic constraint between the sticks. The equations of motion are similar to the former case of one motor advancing on one stick and carrying the other, except for the kinematic constraint (2.10) which is different. Here, the point of motors connection moves on both sticks. Since the variations between kinesin motors are not large, we will assume that both motors advance on the stick with the velocity u:

(2.12)
$$\mathbf{V}_{gc1} + \boldsymbol{\omega}_1 \times \boldsymbol{\chi}_1 + u [\cos \theta_1, \sin \theta_1] = \mathbf{V}_{gc2} + \boldsymbol{\omega}_2 \times \boldsymbol{\chi}_2 + u [\cos \theta_2, \sin \theta_2]$$

with the same notation as in (2.7) and (2.8).

Solving the equations shows that this interaction is highly symmetrical. As can be seen in Figure 14, the sticks are opening and closing again, and the final angle is identical to the initial angle. Figure 15 depicts the angle between the sticks as a function of time for the case of $l_1 = l_2 = 1$, $\theta_{i1} = \pi/3$, $\theta_{i2} = 0$, $\chi_1 = -1/2$, $\chi_2 = -1/2$.

In this interaction, considering different motor properties similar to the suggestions in the previous section will not brake the symmetry, since the free rotation between the sticks emerges from the connection between the two motors, which in the experimental works was a simple biotin-streptavidin connection (a simple string that is able to rotate freely).

The symmetry of this interaction makes it irrelevant to the formation of arrangement of the sticks. This result is in contrast to former works [23], in which the two motors - two sticks interaction induced alignment of the sticks. The difference arises from the different modeling of the connection point between the motors and sticks. While in [23] the connected motors were simulated as an elastic spring, our model assumes a moving connection point allowing free-axis rotation, which enabled large influence of the hydrodynamic drag on the sticks angles.



Figure 14: Interaction of two sticks connected by two connected motors, position in different times. The red point marks the interaction point.





2.2.3 <u>3 sticks – closing triangle</u>

Interactions between more than two sticks connected by motors can lead to forces that will cause the motors to detach from the sticks or stop advancing. We calculated the case of a triangle made of three connected sticks, with two of its edges with constant length and one of them shortening. Such case would be the result of a motor advancing on stick number 3 and carrying stick number 2 shown in Figure 16.



Figure 16: Structure of the triangle in different times, as stick 2 advances on stick 3 in the direction of axes zero.

The construction is $l_1 = const$, $l_2 = const$, $l_3 = l_0 - ut$. Stick 1 starts at the origin of the axes, and stick 3 is on the x axis. From the geometric construction we can derive the function for the angle change in time. Starting from the cosine rule $l_3^2 = l_1^2 + l_2^2 - 2l_1l_2 \cos\beta$ and differentiating by time, we obtain:

(2.13)
$$l_3 u = l_1 l_2 \frac{\partial (\cos \beta)}{\partial t}$$

For small angles $\cos\beta = 1 - \frac{\beta^2}{2}$, $\frac{\partial(\cos\beta)}{\partial t} \approx -\beta\dot{\beta}$, therefore:

(2.14)
$$\frac{ul_3}{l_1 l_2} = -\beta \dot{\beta} \Longrightarrow \quad \dot{\beta} = -\frac{ul_3}{l_1 l_2 \beta}$$

For $\beta = 0$, $l_3^2 = l_1^2 + l_2^2 - 2l_1l_2 \Rightarrow l_3^2 = (l_1 - l_2)^2$. If $l_1 = l_2$, then $\dot{\beta} \propto -u$ and β approaches zero linearly, as shown in Figure 17a. If $l_1 \neq l_2$, then the denominator of (2.14) approaches zero while

the nominator does not, resulting in a very fast change of the angles when the motor approaches the end of stick 3, as shown in Figure 17b. Such fast movement will result in very strong torque on the motor, thus forcing it to detach from the stick and causing the triangle to fall apart.



Figure 17: Angles change as a function of time. Red $-\dot{\alpha}$ (below blue), Green $-\dot{\beta}$, Blue $-\dot{\gamma}$.(a) for $l_1 = l_2$ (b) $l_1 > l_2$.

For triangles with $l_3=1$, and height 1, the x location of the vertex between sticks 1 and 2 determines the triangle form. For x=0.5 the triangle is an isosceles triangle, as shown in Figure 18.



Figure 18: Triangles with $l_3=1$ and height 1, for different locations of the vertex between sticks 1 and 2 (purple dot). Solid line - x=0.5, dashed - x=2, dot-dashed - x= -0.5.

Figure 19 displays the angle change $\hat{\beta}$ as a function of the x location of the vertex between sticks 1 and 2, at times close to the arrival of the motor to the end of stick 3. As expected, when the edges are in different lengths, the angle change diverges when the sticks are close to closing.



Figure 19: Change of β as a function of the x location of the vertex between sticks 1 and 2, for $0.9t_m$, $0.99 t_m$, and $0.999 t_m$, when t_m is the arrival of the motor to the end of stick 3.

2.2.4 <u>Regular polygons composed of N sticks, each pulled by one motor</u>

Moving to assemblages with large number of sticks, the general case of N sticks in a regular polygon was solved, each stick pulled by one motor which advances on the next stick. We show how this interaction leads to the formation of a star shape of sticks, and that the hydrodynamic forces dictate a specific trajectory of the sticks motion contrary to the case without any drag.

Stick number n has the following sizes assigned to it:

 \mathbf{R}_{n} - location of the center point of the stick in the lab frame

 V_n - velocity of the point of geometric center (GC) of the stick

(2.15) $\omega_n \hat{z}$ - angular velocity around the point GC \mathbf{F}_n - Force employed on the stick by the fluid $T_n \hat{z}$ - torque employed on the stick at its GC

We will leave the forces and torques as unknown and solve for them using constraints on the velocities. The equations for each stick are:

(2.16)
$$\begin{pmatrix} F_x(n,t) \\ F_y(n,t) \\ T(n,t) \end{pmatrix} = M(\theta(n,t)) \begin{pmatrix} v_x(n,t) \\ v_y(n,t) \\ \omega(n,t) \end{pmatrix}$$

Since there is no external force, the sum of forces and torques is zero:

(2.17)

$$\sum_{n=1}^{N} F_{x}(n,t) = 0$$

$$\sum_{n=1}^{N} F_{y}(n,t) = 0$$

$$\sum_{n=1}^{N} \left[T(n,t) + \left(\mathbf{R}(n,t) \times \mathbf{F}(n,t) \right)_{z} \right] = 0$$

Using the sum of forces we can develop the sum of torques:

Library

$$\sum_{n=1}^{N} \left[\mathbf{R}(n,t) \times \mathbf{F}(n,t) \right] = \sum_{n=1}^{N} \left[\left(\mathbf{R}(1,t) + \mathbf{R}(n,t) - \mathbf{R}(1,t) \right) \times \mathbf{F}(n,t) \right] =$$

$$\sum_{n=1}^{N} \mathbf{R}(1,t) \times \mathbf{F}(n,t) + \sum_{n=1}^{N} \left(\mathbf{R}(n,t) - \mathbf{R}(1,t) \right) \times \mathbf{F}(n,t)$$

$$\sum_{n=1}^{N} \mathbf{R}(1,t) \times \mathbf{F}(n,t) = \mathbf{R}(1,t) \times \mathbf{F}(1,t) + \sum_{n=2}^{N} \mathbf{R}(1,t) \times \mathbf{F}(n,t) =$$

$$\mathbf{R}(1,t) \times \left(-\sum_{n=2}^{N} \mathbf{F}(n,t) \right) + \sum_{n=2}^{N} \mathbf{R}(1,t) \times \mathbf{F}(n,t) = -\sum_{n=2}^{N} \mathbf{R}(1,t) \times \mathbf{F}(n,t) + \sum_{n=2}^{N} \mathbf{R}(1,t) \times \mathbf{F}(n,t) = 0$$

So that

(2.18)
$$\sum_{n=1}^{N} T(n,t) + \sum_{n=1}^{N} \left(\left(\mathbf{R}(n,t) - \mathbf{R}(1,t) \right) \times \mathbf{F}(n,t) \right)_{z} = 0$$

3N equations originate from the resistance matrix, and 3 equations from the sum of forces. However, there are 6N variables which are $F_x, F_y, T, V_x, V_y, \omega$, for each stick. Therefore, equations for the velocities of the sticks as a function of the velocities of stick number 1 are needed: $[v_x, v_y, \omega](n,t) = function(\mathbf{v}(1,t), \omega(1,t), \theta(1,t)).$

To find this function, the velocity constraints the motors employ on the stick are used. We discuss the case where on stick *n* there is one moving motor, which advances on the stick at a constant velocity *u*, and carries stick number n+1. The connection point of stick n+1 to the motor is fixed.

Each stick has 3 "interesting" points:

O – its center point.

P – the point where stick *n* is connected to the motor carrying it on n+1. This point is fixed in time.

 $\chi(t)$ - the point where a motor which advances on stick *n* is located. This motor carries stick *n*-1. The location of this point of the stick is changing in time according to:

(2.19)
$$\chi(t) = \chi_0 + ut,$$
$$-\frac{l}{2} \le \chi \le \frac{l}{2}$$
$$t_{end} = \frac{1}{u} \left(\frac{l}{2} - \chi_0\right)$$

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for a stick with length *l*.

The velocity of point P of stick *n* is combined from the velocity at which it is carried on stick n+1, and the velocity of the point of the stick n+1 where it is connected:

(2.20)
$$\mathbf{v}_{p}(n) = u \left[\cos(\theta_{n+1}), \sin(\theta_{n+1}) \right] + \mathbf{v}_{\chi}(n+1)$$

From equation (2.4), the velocities of the points O and χ are:

(2.21)
$$\mathbf{v}_{\chi}(n) = \mathbf{v}_{o}(n) + \omega_{n}\hat{\mathbf{z}} \times \boldsymbol{\chi}_{n}$$
$$\mathbf{v}_{o}(n) = \mathbf{v}_{p}(n) - \omega_{n}\hat{\mathbf{z}} \times \mathbf{P}_{n}$$
$$\boldsymbol{\chi}_{n} = \boldsymbol{\chi} [\cos \theta_{n}, \sin \theta_{n}]$$
$$\mathbf{P}_{n} = P [\cos \theta_{n}, \sin \theta_{n}]$$

In a regular form, the relations between the angles of the sticks are fixed according to the number of sticks N. The angular velocity of all the sticks is equal, and the locations of the center of each stick are known relative to stick 1, thus allowing the solution of the system of equations.

(2.22)

$$\theta(n,t) = \theta(1,t) + \frac{2\pi}{N} (N-n+1)$$

$$\omega(n,t) = \omega(1,t)$$

$$\mathbf{R}(n,t) = \mathbf{R}(n-1,t) + \mathbf{P}_{n-1} - \chi_n$$

Figure 20 and Figure 21 display the dynamics of four connected stick obtained using the derivation above. Figure 20 shows the location of the sticks in time as they rotate and close. Figure 21a shows the path of the ends of the sticks and Figure 21b the direction of the forces on their geometric centers.



Figure 20: Locations of four closing connected sticks at different times.



Figure 21: (a) Path of the ends of 4 connected sticks in the XY plane. (b) Direction of the forces on the geometric center of the sticks in the XY plane. The force on stick 1 in t=0-0.1 is marked in black.

A problem with similar kinematic constraints as the problem of connected sticks, but much easier to solve, is the problem of cyclic pursuit of points in the plane (e.g. [29]). Here, N points are moving with velocity u, where the velocity of point n is in the direction of point n+1. This problem can be regarded as the motion of N connected sticks moving without any drag, where stick N is the line connecting the points n and n+1. In order to work with the same geometric constraints as the problem regarded above, the initial locations of the points were at the vertices of regular polygons.

Figure 22 displays the path of the ends of the connected sticks with hydrodynamic drag (full lines), compared with the path of points in cyclic pursuit. It can be seen that the basic formation,

as well as the final star shape structure, is controlled by the geometry of the sticks connections. However, the hydrodynamic forces dictate the specific trajectory of the sticks' motion.



Figure 22: Path of the ends of the sticks in the XY plane. Full lines - the trajectories of the sticks' ends rotating in a low Re medium. Dashed lines – trajectories of points in cyclic pursuit, which can be regarded as the ends of sticks rotating without drag.

2.3 <u>Summary</u>

This chapter investigated the flow-driven re-orientation of sticks moving in low Reynolds number medium driven by molecular motors, with the aim of finding alignment and order mechanisms. In our model, the motors are represented by rigid constraints, allowing free (frictionless) rotation of the sticks around the interaction point. This modeling introduces more influence of the viscous forces on the dynamics of the sticks compared to previous works. The key result of this part is the analysis of the interaction between two connected sticks, with two possible connection types considered. Contrary to former works, we showed that in our model, the interaction of a motor which advances on two sticks is highly symmetrical and does not lead to sticks alignment. However, such alignment is possible due to an interaction which was not considered before, in which a motor is advancing on one stick and carrying the second (immobile) stick. We investigated different possible motor properties, and concluded that in order to induce alignment the propulsion velocity of the motor on stick should vary with the angle or the angle change, while motors should possess random attachment/detachment kinetics.

We continued with the consideration of larger assemblages of sticks, which provided nice examples of combined influence of geometry and hydrodynamic forces on sticks organization. The problem of a triangle of sticks with a motor advancing on one of the triangle's sides and carrying another was analyzed. We concluded that in non – isosceles triangles, as the motor approaches the end of the triangle's side, the pulling force on the motor will be very strong, leading to its detachment and causing the triangle to fall apart. Lastly, the dynamics of regular polygons composed of N interconnected sticks was considered, showing the formation of a star shape, and demonstrating now the hydrodynamic drag changes the connected sticks motion relative to the case without drag.

We conclude that the mechanism of a single motor connected to two sticks is a nonsymmetric interaction, which can create alignment and order in an originally isotropic layout of rods. Although it is not a very efficient mechanism, it is a possible process participating in the microtubules alignment phenomena observed experimentally.

3 Swimming of finite filaments

This chapter details the work on the subject of undulatory swimming of finite-length filaments⁶. The work detailed here was published in [30]. First we bring the background relevant to this problem, including basic properties of swimming in low Re medium, discussing previous works on the subject and metrics used to rate different swimmers. Also, the mathematical methods which we used to solve the swimming problem are described, followed by the biological background concerning the nematode *C. elegans*. In the second part of this chapter, the derivations and algorithms developed in this work are described. These include the adaptation of the particle-based numerical algorithm to the problem of swimming filaments, the numerical algorithm for the solution of a finite swimming filament in plane motion in the Resistance Force Theory (RFT) method, and the mathematical derivation of the swimming of an infinite filament in RFT. Lastly (3.3), the results concerning the swimming of short filaments are presented, including unidirectional and plain motion, comparison between the results of particle-based computations and the predictions of the RFT method, and comparison to biological swimmers. Specifically, the swimming of *C. elegans* is calculated using the particle-based algorithm. Section 3.4 summarizes the subject of filament swimming.

3.1 Swimming problem background

3.1.1 Swimming in low Re

An important field in low Reynolds hydrodynamics deals with the problem of self-propulsion [31]. It is relevant mostly to small organisms swimming in water, since the dimensions of microorganisms (of the micron scale) causes their advancement in water to be a low Re problem. This problem have been studied since the 1950's with important works by Lighthill [32], Hancock [33] and others, which led to the development of solution methods such as the RFT discussed later on (section 3.1.40) and more advanced slender body theories. The problem gained publicity with Purcell's speech and paper "Life at Low Reynolds Number" [34] where he described clearly the swimming problem and the corresponding "scallop" theorem as follows: swimming is the deformation of the swimmer's surface in time, leading to net advancement of

⁶ This part was done in collaboration with Dr. Oded Keneth.

the body. Since Stokes equations governing the motion are linear and time independent, there is no significance to time and the swimming problem becomes a purely geometrical one. In such a media, a sequence of deformations which is reciprocal does not generate net translation⁷. A swimmer which has only one degree of freedom, such as a scallop which can only close and open its shell, can only do reciprocal motion and therefore cannot swim in low Re media. A swimmer with two degrees of freedom, such as the 3-link swimmer suggested by Purcell, is capable of doing a non-reciprocal motion and therefore will advance. Both the scallop and the 3-link swimmer are depicted in Figure 23. Although introduced by Purcell in 1976, the direction of motion of the 3-link swimmer was calculated only at 2003 [1, 2], concluding that the direction is dependent on the angular amplitude of the swimming strokes as well as on the relative length of the links. This demonstrates the non-intuitive nature of low Re swimming.



Figure 23: (a) a scallop which has only one degree of freedom cannot swim in low Re medium [34]; (b) Purcell's three link swimmer.

There are many swimming strategies employed in nature and suggested theoretically. Among those are the cilia, the filament swimming, and the ameboid. A cilia is the beating of two to many small arms, and an ameboid is a non – filament body which deforms in order to advance [36-38]. In nature, long filaments advance through helical rotation such as *E. coli* or spirochete [39], or by two dimensional undulations such as sperm cells and nematodes. Both options are presented in Figure 24.

⁷ Reciprocal sequence means that it transforms from form A to B, and then transforms back by time reversed deformations.



Figure 24: (a) filament swimming by traveling wave; (b) helix swimming through helical rotations.

In this work we focus on swimming due to two dimensional undulations of a finite filament. The problem of infinite filament swimming has been researched by Lighthill [32] which characterized the velocity and swimming efficiency of the filament swimming due to the passage of periodic waves. The swimming efficiency is defined accurately later on, see 3.2.2.1, and for now can be regarded as the total energy expense effectively used in moving forward. For an infinite filament, the shape giving maximum swimming efficiency is one for which the angle between the local tangent to the filament and the swimming direction is constant. In two dimensions, this forces the filament to a non-smooth sawtooth shape. This result extends to finite filaments occupying many undulations of the bending wave, for which the pitching is negligible. For a sinusoidal swimmer, the optimal swimming also employs many small waves. We discuss the comparison of swimmers in the next section where we'll also bring in more details the result of Hancock [33] for the infinite swimmer.

Finite filament swimming has been studied numerically in [40-43] by Resistive Force Theory (RFT), which is a method used for very slender filaments. It assumes that the force distribution along the filament is dependent only on the local velocity, and proportional to the parallel and perpendicular components of the velocity with constant proportionality factors (section 03.1.4). RFT is one of the methods we will use for the solution of finite filaments propulsion. Slender body theory, which is a more accurate method, assumes that the force exerted on the fluid at the surface of the body may be approximated by a distribution of stokeslets along the axis. It has also been used for the investigation of finite filament swimming [40,44,45].

More recent works include the study of finite and infinite filament swimming using RFT, e.g. by Spagnolie and Lauga [46]. They proposed a different optimization function and found the appropriate form of optimal waves (more on that in the next section).

Tam and Hosoi [47] used RFT to find the most efficient stroke for a sperm cell. They started from several seed strokes and found the optimal stroke. They found that the optimal stroke for a sperm cell is a series of symmetrical undulatory bending waves with localized regions of high curvature, which form at the base of the head and propagate towards the end of the flagellum.

Koehler at al. [48] explored toy models of undulating finite-length filaments. They used RFT to calculate the swimming of short filament undulating by sine waves, curvature sine waves (where the curvature of the filament is changing according to a sine wave), sawtooth waves and square waves. The performance of the swimmer was measured according to three metrics, the swimming efficiency, the speed, and the speed at constant power, as explained in the next section. Parametric plots of the performance were presented for each of the wave functions. For all the undulations strategies except the square wave, it was found that the best parameters in all the performance matrices are at the limit of many short waves per filament, similar to the infinite filament. They describe "swimming resonances" which are local maxima in the performance, and find that they occur for specific values of half integer waves (1/2, 3/2,...) and close to minima of the pitching angle. We found similar local optima using RFT (Figure 31). However, the more accurate algorithm we employed (particle-based calculation) shows only one global maximum, implying that these local optima might occur only in very slender filaments.

3.1.2 <u>Comparison between different swimmers</u>

There have been several suggestions in the literature on the comparison method of different swimmers [32,49-51]. Since Stokes equations are time independent, we need to consider a time independent measurement, compensating for the possibility of a swimmer to make faster undulations. One possibility is the normalized velocity, U/c, averaged over a stroke, where $c = \Omega/k$ is the wave speed, Ω being the angular frequency of the wave.

A different metric used extensively to compare different swimmers is the swimming efficiency, which is the work expended in dragging a passive filament divided by the work invested in swimming, $\delta = \frac{\mathbf{F} \cdot \mathbf{U}}{\langle \mathcal{P} \rangle}$, where \mathcal{P} is the rate of dissipation. Maximizing the efficiency leads to maximum swimming speed per mechanical energy, hence allows the maximum advancement if the energy budget is limited. This measurement is important for artificial swimmers, which presumably have limited energy resources. For biological swimmers, however, it is debated whether the power invested in swimming is of importance. Experiments and supporting predictions for flagellated bacteria, such as *E. coli*, show that viscous dissipation accounts for only a few percent of their metabolic costs [34,49,52].

We can assume that body structure and muscle power limit the possibility of organisms to increase their undulation frequency. For example, increasing the solvent viscosity by 10,000 fold decreases the undulation frequency of *C. elegans*, and limits it from approximately 2 Hz down to less than 0.3 Hz [53,54]. In such terms, the only way to swim far is to optimize the waveform, thus making D, the distance per stroke, an appropriate metric to consider.

In the recent works discussed before, there have been a few suggestions of different metrics. Spagnolie et al [46] expanded the definition of efficiency by taking into account the cost of bending, sliding of internal microtubules and internal viscous resistance. According to this definition, the shape of the optimal waves for finite and infinite swimmers changes from sawtooth to sinusoidal waves depending on the cost of bending considered.

Koehler at al. [48] suggested a different speed metric – speed at constant power – which is the ratio of the net speed of the filament operating at constant power to the speed of the same filament when it is pulled at the same power in a straight position. This definition overcomes the problem of inefficiency of undulations with a constant wave speed, which for short filaments leads to large fluctuations in the speed and power of the swimming. Also, Yang at al [55] used a criterion called the "fuel mileage" in their study of Spiroplasma swimming, which is the distance traveled per energy consumed. They considered both internal and external energy in the calculation.

It is instructive to see the predictions of RFT for an optimal infinite swimmer for the swimming efficiency compared with the metric of distance per stroke. From [33] the

approximate expression for the velocity of an infinite filament propagating a plain sinusoidal wave is shown in equation (3.1),

(3.1)
$$\frac{U}{c} \approx -\frac{1}{2} (kb)^2 \frac{\xi - 1}{1 + \xi (kb)^2 / 2}$$

where $c = \Omega/k$ is the wave speed, Ω is the angular frequency of the wave, f_{\perp} and f_{\parallel} are the normal and longitudinal viscous drag coefficients, respectively, and $\xi = f_{\perp}/f_{\parallel}$. According to this solution, the maximum scaled velocity is achieved at $kb = (2/\xi)^{1/2} \approx 1$, with the value of $U/(\Omega b) = -\frac{1}{2}kb\frac{\xi-1}{1+\xi(kb)^2/2} \approx -\frac{1}{4}$ for $\xi = 2$ appropriate to an infinite swimmer. The minus

sign indicates that the swimmer advances in the direction opposite to the traveling wave. According to this, increasing the amplitude of the wave while keeping the frequency constant will result in faster propulsion, as long as kb is maintained at its optimal value. For a finite filament, increasing b while maintaining kb results in fewer waves on the filament, thus making the infinite results less applicable and increasing the pitching which can reduce the forward advancement of the swimmer. From this we expect that for a finite swimmer there will be a global maximum with b and k values optimizing the advancement.

For the swimming efficiency the situation is a bit different. Here, RFT predicts that there is a value of $kb \approx 1.208$ which gives the efficiency optimum with the value of $\delta \approx 8.2\%$, however there is no preference for high amplitude. On the contrary, in order to resemble an infinite filament and keep the pitching at minimum, the best waves for a finite filament are short small amplitude waves. Therefore, the maximum is expected to be at the highest *k* value available.

In our work, the performance of a finite swimmer is measured in both metrics; the swimming efficiency, which is the energy dissipated in swimming a fixed distance at a fixed speed, and the distance per stroke. We find the optimal parameters for a sine wave undulation for each metric, and display the differences between simulations in the RFT method and the more accurate particle-based algorithm. We find that while the most efficient swimmer's parameters are on the line of the optimal kb for an infinite swimmer, the parameters for the sine wave advancing the maximum distance per stroke are quite different from the infinite swimmer's optimal swimming

gait. The particle-based algorithm and RFT method employed for these calculations are described in the following sections.

3.1.3 Particle-based algorithm

Calculation of the flow around arbitrary clusters of spheres suspended in viscous fluid is useful for many areas, and was done in different methods over the years [56-58]. Filippov [59] has demonstrated a numerical algorithm allowing the solution of the hydrodynamic resistance and the flow field around clusters of spheres. In this algorithm, Lamb's fundamental solution of the Stokes' flow outside a single sphere is generalized to the case of N_p non-overlapping spheres of arbitrary size with no-slip boundary conditions. The velocity is expanded in a series of solid spherical harmonics centered at an individual sphere. The equations for the boundary conditions are also expanded in a series of spherical harmonics truncated at some level \mathcal{L} . Then, the direct origin to origin transformation of spherical coordinates is used, along with the transformation of spherical coordinates. This yields a system of $3 \times N_p \times \mathcal{L} \times (\mathcal{L}+2)$ linear equations for the expansion coefficients, which are solved numerically. The method was tested by comparison with theoretical and experimental data.

The original algorithm was developed with the question of hydrodynamic properties of fractal clusters in mind. It has been later adjusted for the solution of various swimming problems, such as Purcell's torodial swimmer, with cargo [36] and without cargo [60], and the swimming of helical filament in heterogeneous viscous media [39]. A similar approach was used in [61] for the calculation of a large variety of different swimmers.

Here, we shall use this algorithm to solve the motion of a swimmer made of beads. This necklace undulates in a sinusoidal wave (section 3.2.2). In this method, the hydrodynamic interactions between different parts of the filament are described accurately, which leads to different results than predicted by the RFT method. However, this method demands a longer computer time thus allowing fewer computations. The algorithm is brought in the appendix in section 4.1 as developed in [59] and corrected by A. Leshansky.

3.1.4 <u>RFT method</u>

RFT method has been first suggested by Gray and Hancock [33] for the solution of the swimming of infinite-length undulating filaments. It has been used intensively since in the investigation of various swimmers propulsion, including finite undulating swimmers [46] and other forms such as Purcell's swimmer [35]. The basic assumption of RFT is that the moving body is locally slender enough as to neglect the hydrodynamic interactions with other portions of the body. Thus the force distribution along the filament is dependent only on the local velocity, and proportional to the two components of the velocity,

$$\mathbf{f} = f_{\perp} \mathbf{v}_{\perp} + f_{\parallel} \mathbf{v}_{\parallel}$$

where f_{\perp} , f_{\parallel} are the corresponding constant drag coefficients and $\xi = f_{\perp} / f_{\parallel}$. The slender body approximation is the limiting case of the RFT, for a body which is infinitely slender, for which $\xi = 2$. For less slender filaments, we have found the appropriate force ratio by comparing between numerical and analytical solutions as shown in section 3.2.4. Detailed derivation of RFT for finite swimmers is presented in section 3.2.2.

3.1.5 <u>Swimming of the nematode *C elegans*</u>

Caenorhabditis elegans is a 1 mm long nematode (round worm) which dwells in soil. It has been chosen to be a model organism for the research of animal development, genetics and neural system development. It is easy to grow, mechanically and genetically manipulate, yet being a multicellular eukaryotic organism, its research can give insights to similar mechanisms in mammals. Since the 1970's *C. elegans* has been researched intensively, and a large database of knowledge has been gathered on it, including cell fate map, neurosystem analysis and generation of various mutants with different characteristics.

Despite naturally living in soil, *C. elegans* is able to swim. Due to its size, the Reynolds number of its motion in water is ~1, making it possible to investigate its swimming using low Reynolds number approximation. The swimming of *C. elegans* is characterized by fast undulations (~1.5Hz), contrary to its crawling which is by slower body motions (~0.2Hz), and these motions has been considered as separate advancement mechanisms ("two gaits hypothesis"). Research in recent years [53,54,62,63], proved that the swimming and crawling

originate from the same propulsion motion, and that the change in frequency, wavelength, and amplitude of the wave with the change in the advancement media is slow and limited (i.e. "a single gait"). This raises the question whether this gait is the optimal solution to swimming in low Reynolds number media.

In [62], the motility of *C. elegans* was investigated experimentally and theoretically in order to estimate the nematode's material properties. The swimming of *C. elegans* was recorded using high speed camera, and its centerline body motion was extracted by image analysis. This experimental deformation function was used in our research as input to a simulated swimmer made of spheres, as described in section 3.3.5. The advancement of the geometrical center of this swimmer was compared with the experimental nematode, and also used to estimate the efficiency of the *C. elegans* swimming.

3.2 Algorithms and Mathematical derivations

3.2.1 Constraints of a finite swimmer

A finite swimmer of length l undulating according to the function y(x) obeys the equation:

(3.3)
$$l = \int_{s_0}^{s_1} (1 + y'(x)^2)^{\frac{1}{2}} dx$$

Where s_0 , s_1 are the limits of the swimmer. For a swimmer propagating a traveling sine wave, $y(x) = b\sin(kx + \omega t)$, one of the realizations is to choose $s_0 = -s_1 = -\pi p/k$, when p is the number of waves occupying the filament and kl the wave number. Thus, there are three mutually dependent parameters characterizing the wave form; kl, b/l and p, and setting the values of two of them dictates the third. Figure 25a shows the relations between the parameters. As the amplitude grows, the number of waves on the filament has to decrease in order for the constraints of the finite length to hold. The relations between kl, b/l and p changes as a function of time. We chose to work with a wave with constant b/l and kl, and let p change during the cycle. We characterized the p value for each stroke by the value of p time-averaged over one period of undulation. At low values of p, the variation can be significant, up to 30% of the mean value at p = 0.2 (Figure 25b). However in the range more relevant to most of our results, at p > 0.5, the standard deviation of p is below 10%.



Figure 25: (a) Contour plots for average p as a function of kl and b/l. The dashed line is $kb \approx 1.2$, the optimal kb for efficiency of an infinite sine wave. The dotted line is $kb \approx 1$, the optimal kb for the velocity of an infinite sine wave; (b) Contour plots of the standard deviation of p during a stroke, in percentage, as a function of kl and b/l.

3.2.2 Particle-based calculations

We solved the problem of the swimming of an undulating filament using particle-based calculations based on the algorithm displayed in 3.1.3. In this approach the hydrodynamic interactions between different parts of the filaments are calculated accurately, thus enabling the simulation of bodies which are not extremely slender. The particle-based algorithm allows the calculation of the flow around an arbitrary array of spheres, and enables the solution of the velocities of the spheres given the forces, or vice versa.



Figure 26: Snapshot of the filament built from $N_p = 30$ spheres of radii a and distance between centers d = 2.02a propagating a plane sine wave.

For the swimming problem, we constructed a swimmer made of N_p nearly touching spheres of radii *a*, as shown in Figure 26. This necklace undergoes a deformation of traveling sine waves, and the linear and angular velocities of its geometrical center are calculated using the particlebased algorithm. Afterwards, the velocities are interpolated and integrated to obtain the angle of rotation and the motion of the swimmer geometrical center (GC) in the lab frame. The method of calculation is detailed in the following, with a few fine details of the implementation discussed in the next section.

One undulation period of the traveling sine wave is divided to time steps, in each time step the spheres are distributed along the centerline which obeys the function $\mathbf{r}_0(s,t) = \{s, b \sin(ks - \Omega t) + Y(t), 0\}$. Here s is a Cartesian coordinate in the body frame of reference. Y(t) includes additions to the deformation function, required to satisfy the incompressibility condition and keep the geometrical center of the filament at y=0. These additions are discussed more thoroughly in section 3.2.2.2. The distance between the spheres centers is d = 2.02a, and the overall length of the filament is $l = (N_p - 1)d + 2a$. The vector of locations of the spheres in each time step is checked to avoid spheres collisions, and used to calculate the linear velocities of the spheres using a second order backwards difference scheme.

The velocity of the ith sphere contains the contributions according to the equations in (3.4). U and $\boldsymbol{\omega}$ are the rigid body translation and rotation velocities for which we wish to solve. \mathbf{u}_i is the deformation velocity found numerically, consisting of transverse undulations and a tangential velocity as the spheres are redistributed along the filament due to the incompressibility constraint. $\boldsymbol{\omega}_i$ is the rotation rate of the ith sphere with respect to the center sphere. It is composed of the rotation due to local bending of the filament and rigid rotation of the whole filament.

(3.4)
$$\mathbf{U}_{i} = \mathbf{U} + \mathbf{u}_{i} + \boldsymbol{\omega} \times \mathbf{R}_{i} + \boldsymbol{\omega}_{i} \times \mathbf{r}$$
$$\mathbf{u}_{i} = (\partial \mathbf{r}_{0} / \partial t)_{i} + \alpha_{i} \hat{\mathbf{s}}$$
$$\boldsymbol{\omega}_{i} = \frac{1}{\gamma} (\hat{\mathbf{s}} \times \partial \mathbf{v}_{0} / \partial s)_{i} + \boldsymbol{\omega}$$

 \mathbf{R}_{i} is the radius vector connecting the GC of the swimmer to the center of ith sphere, \mathbf{r}_{i} is the radius vector with origin at the center of ith sphere, and $\hat{\mathbf{s}}$ is the local unit tangent to the filament centerline at the position of ith sphere. $\gamma = |\partial \mathbf{r}_{0}/\partial s|$, and γds is a length element of the filament centerline. The unknown rigid body translation and rotation are found using the constraints of force and torque free motion:

(3.5)
$$\mathbf{F} = \sum_{i} \mathbf{F}_{i} = 0$$
$$\mathbf{T} = \sum_{i} \mathbf{T}_{i} + \mathbf{R}_{i} \times \mathbf{F}_{i} = 0$$

Where $\mathbf{F} = \{F_x, F_y\}$ and $\mathbf{T} = T_z \hat{\mathbf{z}}$. Here $\mathbf{F}_i = \int_{\partial S_i} \boldsymbol{\sigma} \cdot \mathbf{n} dS$ is the hydrodynamic force and $\mathbf{T}_i = \int_{\partial S_i} \mathbf{r}_i \times (\boldsymbol{\sigma} \cdot \mathbf{n}) dS$ is the hydrodynamic torque exerted on the ith sphere composing the filament. After we calculate the translation and rotation velocities, $U_x(t)$, $U_y(t)$ and $\boldsymbol{\omega}(t)$, respectively, over a period $2\pi / \Omega$, we integrate the interpolated velocities over time to compute the trajectory of the filament in the XY-plane $\mathbf{X}(t)$ and the pitching angle $\boldsymbol{\theta}(t)$:

(3.6)
$$\theta(t) = \int_0^t \omega \, dt$$
, $\mathbf{V} = \mathcal{U}(\theta) \cdot \mathbf{U}$, $\mathbf{X}(t) = \int_0^t \mathbf{V}(\tau) \, d\tau$

Where $\mathcal{U}(\theta)$ is the rotation matrix associated with $\theta(t)$.

From the path in the XY-plane $-\mathbf{X}(t)$, the distance per stroke was calculated according to $D = |\mathbf{X}(T) - \mathbf{X}(0)|$, T being the cycle time. Thus, the initial choice of the x direction does not change the distance per stroke. Moreover, the sideways and rotational movements during the cycle are considered in the calculation of the distance covered per stroke.

3.2.2.1 Power and hydrodynamic efficiency

The power required for our swimmer to maintain its movement is just the dissipation rate $P = \int \mathbf{f} \cdot \mathbf{v} \gamma ds$. The total work in a single stroke is $W = \int_0^T P dt$. This work depends on the specific time parameterization of the stroke. It is well known that the optimal (power-wise) time

parameterization is the one which makes P(t) time independent [35]. Using the optimal

parameterization (specifically $\tau(t) = T \frac{\int_0^t \sqrt{P} dt'}{\int_0^T \sqrt{P} dt'}$) one finds the optimal work to be⁸

$$\mathcal{W} = \int_0^T \mathcal{P} d\tau = \frac{1}{T} \left(\int_0^T \sqrt{P} dt \right)^2$$

It is instructive to look at the *swimming efficiency* δ that measures the energy dissipated in swimming a fixed distance at a fixed speed as

(3.7)
$$\delta = \frac{f_{\parallel} l D^2}{T W}$$

For the steady propulsion it reduces to the standard Lighthill efficiency [32] comparing the power invested in swimming and in dragging the passive filament. For the finite length filament the efficiency in (3.7) can be written as $\delta = \frac{(kl)^2}{(2\pi)^2} \frac{\tilde{D}^2}{\tilde{W}}$, where $\tilde{D} = D/l$ is the distance covered per period and $\tilde{W} = W/f_{\parallel}c^2lT$ is the dimensionless work per period (corresponding to the optimal time parameterization).

The rate-of-work expanded in propulsion of an undulating filament can be found (using the requirement of force- and torque-free propulsion) as $P = \sum_{i=1}^{N} (-\mathbf{U}_i \cdot \mathbf{F}_i - \boldsymbol{\omega}_i \cdot \mathbf{T}_i)$.

Figure 27a shows the deformation function (in blue) along with the actual advancement in the lab frame (in red) of a sine wave with parameters kl = 9.25, b/l = 0.12, $p \approx 0.8$ in different times. Figure 27b depicts the trajectory at the XY plane, and Figure 27c the pitching angle as a function of the time. Figure 27d displays the rate of work during the cycle, normalized according

⁸The fact that $\mathcal{W} \leq W$ may easily be deduced from applying Cauchy-Schwartz inequality. Since the original t-parameterization was arbitrary, this proves that $\tau(t)$ -parameterization is indeed superior to any other.
to $\tilde{P} = \frac{P}{f_{\parallel}lc^2}$. From the rate of work we find the dissipation according to the optimal time parameterization.

The particle-based algorithm described was used to calculate a few different swimming possibilities. First, we calculated one dimensional motion without pitching, where swimmers composed of 30 and 50 spheres were compared. This calculation required 32 time steps per cycle (section 3.3.1). Next, the full two dimensional motion for a swimmer made of 30 spheres was calculated, with the exemption of high kl results for which a swimmer of 50 spheres was used. The 2D motion was more numerically sensitive hence 100 time steps per cycle were used (3.3.2). Lastly, the motion of the nematode *C. elegans* was simulated by a 12 spheres swimmer, using the experimental deformation function of the nematode. This calculation used 55 time steps per cycle, according to the experimental frame rate (section 3.3.5).



Figure 27: (a) In blue, the deformation function of a sine wave with the parameters kl = 9.25, b/l = 0.12, below the motion

Distance between spheres: The distance d = 2.02a was determined by balancing the demand to resemble a unified smooth filament (like a worm), dictating that the spheres should be as close as possible, and the rising accuracy demands arising from very close spheres. The accuracy of the calculation depends on the level of truncation \mathcal{L} of the spherical harmonics functions. For the used d, truncation level of $\mathcal{L}=2$ is sufficient for most calculations, as the difference between $\mathcal{L}=2$ and $\mathcal{L}=3$ is less than 5% even for large undulations. Changing d requires recalculation of the force ratio $\xi = f_{\perp} / f_{\parallel}$ used to compare between the RFT and the particle-based calculations, and

<u>GC correction</u>: A correction to the y-position is required to keep the geometrical center of the filament at y=0. This correction is not important when calculating the overall distance

traveled in a period, since it is averaged over a stroke cycle, but it is important if the velocities and the path in the XY plane are required. The calculation of the location of the filament geometrical center in each time step t_j can be done particle wise, according to $\frac{1}{N} \sum_{i=1}^{N} \mathcal{Y}(r_i, t_j)$, or

by integrating over the theoretical function and satisfying $\int_{s_0}^{s_1} \mathbf{r_0} \gamma ds = 0$. The differences between these approaches are small and completely disappear as N_p increases. The hydrodynamic interaction is not affected by the local structure of the filament, hence it is controlled by the location of the continuous function. Therefore, the more accurate method is the theoretical calculation of GC location, which is indeed what was used in our calculations.

<u>Compressibility condition</u>: The third contribution to the deformation function arises from the compressibility properties of the filament. We chose to simulate an incompressible filament, thereby redistributing the spheres each time step to be in a <u>linear</u> distance d between centers. More accurate implementation of this incompressibility condition would be to calculate the distance d between the spheres according to the length on the filament (i.e. the line integral of the undulation function between centers). However, this approach leads to collisions between spheres in undulations with high curvature. The location of the filament edge is determined in a similar manner. Each time step, the first sphere of the swimmer is located in a distance of half the filament length from the zero on the x axis. From this point, the spheres are distributed according to the deformation function and the incompressibility condition.

3.2.3 Resistance Force Theory for finite and infinite filaments

The results from the particle-based algorithm were compared with analytical and numerical results based on RFT, which neglects the hydrodynamic interactions between different parts of the filament, but allows analytical derivation and fast numerical calculations of the swimming. The following sections display derivations and a numerical algorithm for filament swimming employing local RFT. First, a numerical algorithm for finite filament moving in plane motion is displayed. Later on (section 3.2.3.2) analytical derivation for infinite swimmer is brought. This derivation can be also applied for finite length filament in unidirectional propulsion. Lastly, the calculation of power and hydrodynamic efficiency for the RFT is brought in section 3.2.3.3.

3.2.3.1 **<u>RFT for a finite filament</u>**

The shape of the swimmer at the moment *t* is given by $s \mapsto \mathbf{r}_0(s,t) = (x_0(s,t), y_0(s,t))$, $s_1 \le s \le s_2$. The actual embedding of it in \mathbb{R}^2 is given by $s \mapsto r(s,t) = (x(s,t), y(s,t))$ where

$$\mathbf{r}(s,t) = \mathcal{U}(t) \cdot [\mathbf{r}_0(s,t) + \mathbf{R}(t)], \quad \mathcal{U}(t) = \begin{pmatrix} \cos \theta(t) & -\sin \theta(t) \\ \sin \theta(t) & \cos \theta(t) \end{pmatrix}.$$

The angular velocity of the swimmer is $\boldsymbol{\omega} = \dot{\boldsymbol{\theta}} \hat{\mathbf{z}}$, where dot stands for time derivative, and through some abuse of notation one may write $\dot{\boldsymbol{\mathcal{U}}} = \boldsymbol{\omega} \times \boldsymbol{\mathcal{U}}$. The local swimmer velocity then reads⁹

$$\mathbf{v}(s,t) = \frac{d\mathbf{r}}{dt} = \mathbf{\omega} \times \mathbf{r} + \mathbf{\mathcal{U}} \cdot (\mathbf{r}_0 + \mathbf{R}) = \mathbf{\mathcal{U}} \left(\mathbf{\omega} \times (\mathbf{r}_0 + \mathbf{R}) + \mathbf{r}_0 + \mathbf{R} \right).$$

Here we denote by $\mathbf{v}_0 = \mathbf{r}_0$ the local deformation velocity and by $\mathbf{V} = \mathcal{U}^{-1} \cdot \frac{d}{dt} (\mathcal{U} \cdot \mathbf{R}) = \mathbf{\omega} \times \mathbf{R} + \mathbf{R}$ the extra rigid translation experienced by the swimmer both expressed in a frame rotating with it. We shall denote $\gamma = |\mathbf{r}_0'|$ where prime stands for $\frac{\partial}{\partial s}$. Then $\hat{\mathbf{s}} = \gamma^{-1} \mathbf{r}_0'$ is the unit tangent to the filament as expressed in a frame rotating with it (In the lab frame the unit tangent is $\mathcal{U} \cdot \hat{\mathbf{s}}$.) The local velocity $\mathbf{v} = \mathbf{r}$ can be written as a sum of parallel and transverse velocities, $\mathbf{v} = \mathbf{v}_{\parallel} + \mathbf{v}_{\perp}$ where $\mathbf{v}_{\parallel} = \frac{\mathbf{r} \cdot \mathbf{r}'}{|\mathbf{r}'|^2} \mathbf{r}' = \hat{\mathbf{s}} (\mathbf{V} + \mathbf{\omega} \times \mathbf{r}_0 + \mathbf{r}_0) \mathcal{U} \cdot \hat{\mathbf{s}}$.

We assume that the local force (per unit length) exerted on the swimmer may be expressed as $f = f_{\perp} \mathbf{v}_{\perp} + f_{\parallel} \mathbf{v}_{\parallel}$ for some constant f_{\perp}, f_{\parallel} and denote $\xi = f_{\perp} / f_{\parallel}$. This allows to express the force

⁹ If we work in a frame rotating with the swimmer instead of the lab frame, then the factor \mathcal{U} would drop out from all our equations making them slightly simpler. We refrain doing that to avoid the need for extra notations.

(per unit length) as $\frac{1}{f_{\parallel}}f = \xi \mathbf{v} + (1-\xi)\mathbf{v}_{\parallel}$. Using the above expressions for $\mathbf{v}, \mathbf{v}_{\parallel}$ we obtain that the moving frame force $f_0 = \mathcal{U}^{-1} \cdot f$ is given by

(3.8)
$$\frac{1}{f_{\parallel}} \boldsymbol{f}_{0} = \boldsymbol{\xi} (\mathbf{V} + \boldsymbol{\omega} \times \mathbf{r}_{0} + \mathbf{v}_{0}) + (1 - \boldsymbol{\xi}) \hat{\mathbf{s}} \cdot (\mathbf{V} + \boldsymbol{\omega} \times \mathbf{r}_{0} + \mathbf{v}_{0}) \hat{\mathbf{s}}$$

The zero net force and zero net torque conditions are then

$$\mathbf{F} = \int_{s_0}^{s_1} \boldsymbol{f}_0 \gamma ds = 0, \quad \mathbf{T} = \int_{s_0}^{s_1} \mathbf{r}_0 \times \boldsymbol{f}_0 \gamma ds = 0.$$

Where γds is a length element. At each instant *t* this gives a set of three linear equations for $\mathbf{V} = (V_x, V_y)$ and $\boldsymbol{\omega} = \boldsymbol{\omega} \hat{z}$. Integration over *t* then gives $\theta = \int \omega dt$ which defines the matrix $\mathcal{U}(t)$. The distance covered by the swimmer is found from $\mathcal{U} \cdot \mathbf{R} = \int \mathcal{U} \cdot \mathbf{V} dt$.

In order to compute the advancement of the swimmer, we need to determine the location of the swimmer ends according to the incompressibility constraint. The employment of the incompressibility constraint and the parameterization of the swimmer are discussed in the appendix in section 4.2.

The numerical calculations were performed as follows:

- i. First we fixed numerical values for b, k and ξ (we fixed $\Omega = 1$, l = 1 for all calculations).
- ii. We calculated the expressions for the force and torque densities in the rotated frame f_0 , $\mathbf{r}_0 \times f_0$ by using Eqs. (3.8), (4.8),(4.9). This has three independent components corresponding to the force f_x , f_y and torque n_z densities. We expressed them as $A_{ij}q_j + B_i$, i = 1, 2, 3 where $q = (V_x, V_y, \omega)$.

- iii. We discretized the time range $0 \le t \le T = 2\pi / \Omega$ into N = 100 steps t_i . (Few calculations were done with higher N up to 300.)¹⁰
- iv. For each t_i we first calculated $s_1(t_i)$ by solving numerically Eq. (4.10) which determines the location of the swimmer ends. We then calculated numerically the integrals $A_{ij} = \int_0^{s_i} A_{ij} \gamma ds$, $B_i = \int_0^{s_i} A_i \gamma ds$ and solved $A_{ij}q_j + B_i = 0$ for the values of instantaneous velocities $q = (V_x, V_y, \omega)$. We kept a table containing the values $(t_i, V_x(t_i), V_y(t_i), \omega(t_i)), i = 0, 1, 2, ..N$
- v. Interpolating $\omega(t_i)$ we constructed a continuous $\omega(t)$ which was then integrated to define $\theta(t)$ and hence the matrix $\mathcal{U}(t)$.
- vi. Noting the relation $\mathcal{U} \cdot \mathbf{R} = \frac{d}{dt} (\mathcal{U} \cdot \mathbf{V})$ we constructed the 'rotated frame center of mass velocity' $\mathbf{v}_{cm}(t_i) = \mathcal{U} \cdot \mathbf{V}(t_i)$. We then interpolated it to a continuous $\mathbf{v}_{cm}(t)$ and integrated over t to obtain the trajectory of the swimmer over a cycle. The distance covered per stroke is then $D = \left| \int_0^T \mathbf{v}_{cm}(t) dt \right|$.¹¹

3.2.3.2 **<u>RFT for an infinite filament</u>**

The analysis based on the local RFT for an infinite undulating filament can be found elsewhere (e.g.[32,33]), however we choose to present our short derivation offering a short route to the closed-form expressions for the propulsion velocity and the power dissipated in swimming.

For an infinitely long incompressible undulatory swimmer it is more convenient to use a slightly different representation of the local velocity v_0 , which takes full advantage of the symmetry / homogeneity of the problem. This representation will be slightly different than the

¹⁰ Sometimes we used a slightly larger range e.g. $-0.01 \le t \le T = 2\pi / \omega + 0.01$. Among other things this helps to avoid dealing with removable singularity at t = 0.

¹¹ Some of the described steps are redundant if one is only interested in the final result. These 'redundant' steps however made it easier to inspect for possible errors.

one used in the previous subsection¹² which was better suited to use in numeric. Consider a swimmer powered by traveling wave type undulations, $\mathbf{r}_0(s,t) = \{s, \phi(ks - \Omega t)\}$. Incompressibility then requires \mathbf{v}_0 to be a superposition of movement along the filament $-\alpha(t)\hat{\mathbf{s}}$ and rigid motion (in general a 2D translation and rotation). Due to the geometric nature of low Reynolds swimming one may assume α to be time independent¹³. In the case of the traveling sine wave we take α to be the velocity required to travel along a period of $\mathbf{r}_0(s)$ over time $T = \frac{2\pi}{\Omega}$ i.e.

(3.9)
$$\alpha = \frac{\Omega}{2\pi} \int_0^\lambda \gamma ds = \frac{2c}{\pi} E(-(kb)^2),$$

where $\lambda = \frac{2\pi}{k}$ and $c = \frac{\Omega}{k}$ is the phase velocity. Averaging over the trajectory of a material point we have $\langle -\alpha \hat{\mathbf{s}} \rangle = -c \mathbf{x}$, i.e. the phase speed. Thus $\mathbf{v}_0 = -\alpha \hat{\mathbf{s}} + c \mathbf{x}$ will describe the local velocity due solely to the (incompressible) periodic deformation. For small amplitudes this is just $\mathbf{v}_0 = \{0, -b\Omega\cos(ks - \Omega t)\} + \mathcal{O}(b^3)$.

If we want to describe a swimmer of finite length then we should also specify the parameter range $s \in [s_0, s_1]$. The fact that the longitudinal velocity $(\mathbf{v}_0)_x$ is not exactly zero implies that the location of the edges will contain (small) time dependence $s_0 = s_0(t), s_1 = s_1(t)$. Since the endpoint are material points, $s_0(t)$ and $s_1(t)$ must be solutions of $\frac{ds}{dt} = (\mathbf{v}_0)_x = -\alpha \hat{\mathbf{s}} \cdot \mathbf{x} + c$. This leads to the rather complicated relation $(t_0^{(i)})$ being the integration constants)

$$\mathbf{E}\left(ks_{i}(t) - \Omega t, \frac{(kb)^{2}}{1 + (kb)^{2}}\right) = \frac{\alpha k}{\sqrt{1 + (kb)^{2}}} (t_{0}^{(i)} - t), \ i = 0, 1$$

¹² The two differ by gauge and by time parametrization but are equivalent.

¹³ Making α time independent requires a different choice of time parameterization from the one we used in the previous subsection.

This deviates from the $s_0 = 0$ and Eq. (4.10) for $s_1(t)$ used in the previous section due to the use of different time parameterization and gauge.

Now consider a very long incompressible swimmer described by $\mathbf{r}_0(s,t) = \{s, b \sin(ks - \Omega t)\}$.

The small oscillations of the endpoints, $s_{0,1}(t) = \text{Const} - \frac{b^2 k}{8} \sin(2\Omega t) + \mathcal{O}(b^4)$, are completely negligible compared to *l*. Thus, in the limit of a long swimmer one may take s_0, s_1 as constants and even assume $[s_0, s_1]$ to contain exactly a large integer number *p* of wavelengths. This assumption considerably simplifies the subsequent calculations.

The local velocity due to deformations is $\mathbf{v}_0 = -\alpha \hat{\mathbf{s}} + c\mathbf{x}$ with α given in Eq.(3.9). The total local velocity would include also a rigid motion which for an infinitely long swimmer can only be a longitudinal motion along x-axis, as transverse translation and rotation are zero from symmetry. The total local velocity is then $\mathbf{v} = \mathbf{v}_0 + U\mathbf{x} = -\alpha \hat{\mathbf{s}} + (c+U)\mathbf{x}$ with its longitudinal and transverse components being $v_{\parallel} = -\alpha + (\hat{\mathbf{x} \cdot \mathbf{s}})(c+U)$ and $\mathbf{v}_{\perp} = (\mathbf{x} - (\hat{\mathbf{x} \cdot \mathbf{s}})\hat{\mathbf{s}})(c+U)$, respectively. The corresponding local force on the swimmer is $f \propto \mathbf{v}_{\parallel} + \xi \mathbf{v}_{\perp}$. The transverse component of the force, F_y as well as the torque T_z , vanish by symmetry. The longitudinal force may be expressed in terms of $\gamma = \frac{d\zeta}{ds} = (\hat{\mathbf{s} \cdot \mathbf{x}})^{-1} = \sqrt{1 + (kb)^2 \cos^2(ks - \Omega t)}$ as

(3.10)
$$F_{x} = \int f_{x}d\zeta = \int \left[\xi(c+U) - \alpha\gamma^{-1} + (c+U)(1-\xi)\gamma^{-2}\right]d\zeta = \int \left[\xi(c+U)\gamma - \alpha + (c+U)(1-\xi)\gamma^{-1}\right]ds$$

Requiring $F_x = 0$ determines U. Since the integrand is periodic of period $\lambda = 2\pi/k$ and since the integration range is assumed to be much larger than the wavelength, $s_1 - s_0 \gg \lambda$, one may just integrate over one period $\int_0^{\lambda} (...) ds$. Using the identities in the appendix (section 4.3), the swimming velocity is then found to be

(3.11)
$$\frac{U}{c} = -\frac{(\xi - 1)(E' - K')}{K' + \xi(E' - K')}$$

Here again $c = \Omega/k$, $\xi = f_{\perp}/f_{\parallel}$ and $E' = E(-(kb)^2)$, $K' = K(-(kb)^2)$ where $K(m) = \int_0^{\pi/2} (1 - m \sin^2 \theta)^{-1/2} d\theta$ is the complete elliptic integral of the first kind. The minus means that the filament is propelled in the direction opposite to that of the wave propagation. Note that the expression in (3.11) is a sole function of (E' - K')/K' and using its asymptotic expression $\sim (kb)^2/2$ for small-amplitude undulations, $kb \ll 1$ in Eq. (3.11) yields an asymptotic result which is identical to the approximate solution (3.1) derived in the seminal paper [33]. We note that the expressions (3.1) and (3.11) also have an identical (finite) limit for $kb \to \infty$ and therefore, the two expressions provide quite close estimates of the propulsion speed for an arbitrary value of kb.

Note that even though equations (3.1) and (3.11) were derived for infinite filament where transverse displacements and pitching cancel out due to symmetry, it can be also applied for approximate modeling of finite-length filament unidirectional propulsion where transverse displacement and turning are disallowed.

3.2.3.3 Power and hydrodynamic efficiency in RFT

Our numerical calculation of the swimmer in plane motion allows simple calculation of \mathcal{W} by integrating $\int_0^T dt \sqrt{\int_{s_0}^{s_1} \mathbf{f} \cdot \mathbf{v} \gamma ds}$ and squaring it. For an infinitely long sine wave we have

$$\boldsymbol{f} \cdot \mathbf{v} = f_{\perp} v_{\perp}^{2} + f_{\parallel} v_{\parallel}^{2} = f_{\perp} (U + c)^{2} (1 - \gamma^{-2}) + f_{\parallel} (\alpha - (U + c) / \gamma)^{2}$$

Integrating over s and using Eqs. (3.9), (3.11), we find:

(3.12)
$$P = f_{\parallel} c^2 l \left(\frac{4E'}{\pi^2} - \frac{1}{\xi E' + (1 - \xi)K'} \right) E$$

(Note that $s_1 - s_0 = \frac{c}{\alpha}l$.) Since the result does not depend on t it is clear that $\mathcal{P} = P$ and the total work per stroke is just $\mathcal{W} = PT$. At $kb \ll 1$ the expression in the brackets of (3.12)

asymptotes to
$$\frac{\xi(kb)^2}{\pi} + \mathcal{O}((kb)^4)$$
 and $\mathbf{E}' \approx \frac{\pi}{2} + \mathcal{O}((kb)^2)$, leading to
 $\mathcal{P} \approx \frac{1}{2} \int_{\mathbb{R}} \xi c^2 (kb)^2 l = \frac{1}{2} \int_{\mathbb{R}} \xi (\Omega b)^2 l$.

For infinitely long filament the net work (time parameterization of the stroke does not matter here) per period is $W = \int_0^T P d\tau = f_{\parallel} c^2 l T \tilde{P}(kb,\xi)$, while the distance it covers per period is $D = UT = cT \tilde{U}(kb,\xi)$, yielding $\delta = \frac{\tilde{U}^2}{\tilde{P}}$. Note that in the framework of RFT for either finite or infinite filament both propulsion characteristics, D/l and δ , do not depend explicitly on f_{\parallel} , but are only functions of the ratio $\xi = f_{\perp} / f_{\parallel}$.

3.2.4 Force ratio calculation

The comparison of the local RFT with the results of particle-based simulations requires the knowledge of the ratio $\xi = f_{\perp} / f_{\parallel}$. For slender filaments the corresponding force densities are $f_{\perp} = 2f_{\parallel} \approx 4\pi\mu E + \mathcal{O}(1)$, whereas $E = (\ln 2/\epsilon)^{-1}$ is a small parameter and $\epsilon = 2a/l \ll 1$ is the aspect ratio, while *l* and 2*a* are the length and the typical width of the filament [64]. However, the limiting value of $\xi = 2$ is only achieved for extremely slender (exponentially thin) filaments. For finite length-filaments the value of ξ was determined numerically from computation of the viscous drag exerted on a spheres-built rod composed of N_p nearly touching spheres in the longitudinal and transverse direction. ξ as a function of the rod aspect ratio ϵ is presented in Figure 28 together with the best fit of the form $\xi \approx c_1 \left(\frac{1-c_2E}{1+c_2E}\right)$ (red, solid) suggested by the slender body theory solution [65], where $E = (\ln 2/\epsilon)^{-1}$. For a prolate spheroid $\xi = 2\left(\frac{1-E/2}{1+E/2}\right) + O(\epsilon^2 \ln \epsilon)$, while for a spheres-built rod with the distance of d = 2.02a between spheres we find rather close values of $c_1 = 1.96$ and $c_2 = 0.525$ suggesting that ξ is rather insensitive to the local variation of the filament shape. The formula for the prolate spheroid indicates that ξ approaches the limiting value of 2 in a slow logarithmic rate (see

Figure 28) and in the wide range of slenderness ξ is in the range 1.4–1.6. For $N_p = 30$ ($\epsilon \simeq 0.033$) we find $\xi \simeq 1.51$. This calculation is repeated in section 3.3.3 for different distances between spheres, showing that the form $\xi \approx c_1 \left(\frac{1-c_2E}{1+c_2E}\right)$ remains valid for large variation in d.

For the comparison of the work invested in swimming between the RFT and the particle-based calculation, the parameter f_{\parallel} is required in addition to ξ . For the filament with aspect ratio $\epsilon = 1/30$ we found that $f_{\parallel} \approx 3.3\eta$ yields an excellent agreement between the prediction of the RFT and particle-based simulations for all values of p, in the 2D as well as 1D calculations detailed in the following. For calculations with $\epsilon = 1/50$ the corresponding value was $f_{\parallel} \approx 3\eta$.



Figure 28: Force ratio $f_{\perp} / f_{\parallel}$ as a function of the aspect ratio $\epsilon = 2a/l$. The markers (°) signify numerical calculations for a spheres-built straight rod of length l made of N_p spheres of radii a. The continuous line stands for the best fit, $\xi = c_1(1-c_2E)/(1+c_2E)$, with $c_1 = 1.96$ and $c_2 = 0.525$ ($c_1 = 2$ and $c_2 = 0.5$ correspond to the slender body theory result for a prolate spheroid [65]).

3.3 <u>Results</u>

This section brings the results of our research on the swimming of short filaments. We begin with one dimensional movement, in which the velocity of the swimmer in only in the X direction. For such motion the analytical derivations of the RFT method for an infinite swimmer are applicable (section 3.2.3.2), and are used in comparison with results from the particle-based algorithm to show the validity of the calculations. Next, 2D motion is concerned. Undulations of sine waves with different parameters are searched to find the best swimmer distance and efficiency –wise, and we show the agreement and the difference between the particle-based algorithm, the numerical two dimensional RFT calculations, and the analytic RFT calculations for the infinite swimmer. Contour plots calculated in the RFT method are used to find the parameter space which will give good swimming in both objectives. Turning to more biologically relevant questions, the parameters. Special attention is given to *C. elegans*, and its experimental deformation function is used to calculate the swimming trajectory and efficiency.

3.3.1 Unidirectional motion

The swimming of a filament in one dimensional motion was calculated and compared to the RFT predictions. In this motion the constraint is only on the sum of forces in the x direction, $\mathbf{F}_x = 0$, while the force in the y direction and the torque are not balanced. The velocity of the GC is only in the x direction, so there is no pitching. The 1D motion allows the comparison of the numerical particle-based calculations to the <u>analytic</u> derivation by the RFT, in contrast to the plane motion where the RFT solutions also rely on numerical calculations.

1D calculations were done for swimmers made of 30 and 50 spheres, as presented in Figure 29a and b. Each point is a different calculation of the advancement of a swimmer doing an undulation with prescribed parameters of (kl, b/l). The value of kl during a stroke is fixed, but it is different between points in order to keep the average p fixed on each curve. The average velocity in a stroke is scaled by the wave velocity, while the error bars present the double mean standard deviation of the velocity during the stroke. The solid line corresponds to the approximate solution by Grey & Hancock discussed before (3.1), and the dashed line is the prediction of the 1D RFT in equation (3.11).

As seen in the figures, there is a good agreement in low kb values, but considerable deviation as kb grows, a deviation which starts sooner in higher p values in which the filament contains more waves and there are more interaction inside the filament. Going to slender filaments increases the agreement, as expected and shown in the calculation of a swimmer made of 50 spheres, where the deviation starts in higher values of kb. The 1D dissipation was also calculated and shows good agreement between the RFT derivation (3.12) and the particle-based calculation, as depicted in Figure 29c, using the same value of the parameter f_{\parallel} as used for the 2D calculations (as explained in 3.2.4).



Figure 29: Scaled propulsion speed, averaged over time of a period $\langle U \rangle / c$ plotted vs. kb for a filament undergoing 1D locomotion opposite to the direction of wave propagation (forbidding pitching and transverse motion). Different *p* values are displayed in different p = 0.7to p = 2.from colors, The bars size is doubled mean standard deviation of the velocity from its mean during the period of undulation. The dashed line corresponds to the prediction of the RFT in (3.11), the solid line corresponds to the approximate solution (3.1). (a) Filament composed of 30 spheres corresponding to $\xi = 1.51$ in RFT expressions; (b) filament composed of 50 spheres, corresponding to $\xi = 1.56$ in RFT expressions; (c) optimal work per period, $\mathcal{W}/f_{\scriptscriptstyle \parallel}c^2 lT$. The solid line corresponds to the prediction of the RFT in (3.12)

3.3.2 <u>Two dimensional motion</u>

For a two dimensional motion, we compared the numerical calculations using the particlebased algorithm and the numerical calculations done with the RFT method. This comparison indicates when the local interactions are important. We expect the local interactions to be negligible when the filament is very slender, $\kappa a \ll 1$, where $\kappa = |\partial^2 \mathbf{r_0} / \partial s^2|$ is the local curvature of the filament centerline. For our deformation function $\mathbf{r_0}(s,t) = \{s,b\sin(ks - \Omega t) + Y(t),0\}$ $\Rightarrow |\partial^2 \mathbf{r_0} / \partial s^2| = |bk^2 \sin(ks - \Omega t)| \le bk^2$. Hence, the local RFT should hold while $abk^2 \ll 1 \Rightarrow kb(kl) \ll \frac{1}{a} = 2\epsilon^{-1}$. Our actual comparisons between the RFT and particle-based results, shown in the following figures, found the line of RFT validity to pass at $kb(kl) \approx 0.5\epsilon^{-1}$.

Figure 30a-c displays the particle-based and RFT results for lines of constant average p. Each point is a calculation in which the kl value is constant through the swimming stroke, however from point to point kl is different as needed to keep the value of average p constant. Figure 30d-f depicts the results in curves of equal kl, while the average p changes from point to point. This presentation allows the sampling of higher amplitude waves. Figure 30a and d present the scaled distance the swimmer advances in one stroke as a function of the amplitude. For each p value there is optimal amplitude with maximum distance, and the optimal parameters distance-wise are $p \approx 0.8$, $b/l \approx 0.24$, and $kl \approx 8.86$, for which $D/l \approx 0.1167$. The agreement between the RFT and the particle-based calculation is very good at low values of kl, as can be seen in Figure 30d, but as kl increases, the deviation between the methods starts at lower amplitudes. In high kl and b/l values, the RFT neglect of the inter-filament interactions leads to overestimation of the distance per stroke. Figure 30b and e display the maximum pitching angle during the stroke vs. the amplitude b/l for the same values of p and kl as in Figure 30a and d correspondingly. The maximum pitching angle is twice the angle between the mean direction of propulsion and the initial orientation of the swimmer at t=0. It indicates how much the swimmer advances "sideways" instead of "forward", and a reasonable assumption was that substantial pitching will reduce the overall advancement of the swimmer. As can be seen in Figure 30b, low p values lead to high pitching angle, which decreases when the number of waves increases, as expected, since for large number of waves there is no turning at all. Contrary to our assumption,

the maximal distance is achieved with substantial turning of $\theta_m \approx 53^\circ$. The agreement between the RFT and the particle-based computation is very good for most values of *p* and *kl*, except for high *p* values where the curvature is high and reduces the accuracy of the RFT assumptions. Overall the agreement between the methods is better for the angle calculations than for the distance results. We argue that since the pitching angle is just the maximum of the integral over the angular velocity, while the traveled distance combines translation and pitching, the latter is expected to be more sensitive to the intra-filament hydrodynamic interaction.

Figure 30c and f display the net work per period dissipated by viscosity, corresponding to optimal time parameterization as discussed earlier (section 3.2.3.3), vs. the scaled amplitude. The agreement between the methods is very good, although requiring an additional parameter f_{\parallel} as discussed before (section 3.2.4). It can be seen that for the same value of b/l less energy is dissipated by working in low values of p and kl, when there is less relative motion between parts of the filament. In high kl values the energy growth is more moderate, in a value of b/l corresponding to undulations with less than half a wave ($p \approx 0.5$). At large amplitudes the RFT underestimates the power, a deviation which increases as kl grows.

Figure 30 (next page): Comparison of the particle-based simulation results vs. the predictions of the RFT for a finite length filament with aspect ratio $\epsilon = 1/30$.

(a) – (c) For fixed values of the mean number of waves p; the corresponding mean p values are shown. Symbols correspond to the results of particle-based simulations: p = 1.4 (\Box), p = 1.2 (\triangleleft), p = 1 (∇), p = 0.8 (\circ),

p = 0.7 (>), p = 0.6 (\diamond) and p = 0.4 (Δ); the solid lines are the prediction of the RFT with $\xi = 1.51$.

(d) – (f) For fixed values of the wave-number $kl : 2 (\Box)$, 4 (°), 6 (<), and 9.25 (>). The upper (filled) triangles (\blacktriangle) correspond to kl = 14 computed for a longer filament with aspect ratio of $\epsilon = 1/50$. The continuous lines stand for the prediction of the RFT with $\xi = 1.51$ (corresponding to $\epsilon = 1/30$, solid lines) and $\xi = 1.56$ (corresponding to $\epsilon = 1/50$, dashed line).

(a) and (d): scaled distance per period of undulation, D/l vs. the scaled undulation amplitude b/l.

(b) and (e): maximum pitching angle during a stroke $heta_m$, vs. the scaled amplitude b/l .

(c) and (f): optimal work per stroke, $\xi = 1.56$, vs. the scaled amplitude b/l.



1.4

1.4

1.4

3.3.2.1 Efficiency calculations

Using the displacement per stroke and the power invested in a stroke we can calculate the swimming efficiency, defined as $\delta = \frac{f_{\parallel} l D^2}{TW}$. The efficiency for an infinite swimmer can be found from the analytical RFT results developed in section 3.2.3.3.

For a swimmer with $\xi = 1.515$, which fits a slenderness of $\epsilon = 1/30$, there is an optimal kb value, kb = 1.29, which gives the maximum efficiency. For this value of kb we calculated the efficiency using RFT method for a 2D filament with the same ξ . Figure 31 depicts the maximum efficiency for these parameters (3.32%) in dashed red line, and the efficiency calculated using the RFT method for a finite filament (blue) vs. the wave number kl. Indeed as the wave number increases there are many short waves on the filament, similar to an infinite filament and its efficiency converges to the efficiency of an infinite filament. However the convergence is not monotonic, and there are local maxima at relatively low values of kl. The green line displays the pitching angle, and the dashed grid lines demonstrate how the maxima in δ coincide exactly with zeros of θ_m . Similar local maxima were demonstrated in [46] and [48]. Like them, also in our case these maxima occur at values near 1.5 waves on the filaments. The average p values are 1.42, 2.46, and 3.47, close to the values of 1.5, 2.5, 3.5 viewed at the former works. Unlike [48], there is no effect of the movement of the GC (bobbing), and the efficiency maxima are exactly at θ_m zeros. However, in results from the particle-based calculations conducted for a swimmer with aspect ratio 1/30, (□ and ∘ in Figure 31), there is only one global maximum of the efficiency. Calculations for a swimmer with aspect ratio 1/50 show similar results. This indicates that the local maxima observed in the RFT results are relevant only for very slender filaments.



Figure 31: In blue, hydrodynamic efficiency in percentage, δ , vs. kl from the RFT for a finite filament with $\xi = 1.51$ for fixed kb = 1.29 corresponding to the optimal efficiency of infinite filament with the same ξ , in dashed red. The green line displays the maximum pitching angle in the RFT. The black squares (\Box) and the green circles (\circ) are the efficiency and the maximum pitching angle in the particle-based computations, respectively. The values of average p at the efficiency maxima are 1.42, 2.46, and 3.47.

Figure 32 depicts the efficiency calculations of the 30 spheres swimmer vs. the amplitude, for p and kl as in Figure 30, and two higher kl values. As can be seen, the efficiency grows with kl and p, but reaches a maximum of $\delta \approx 2.8\%$ at relatively low values of $kl \approx 9.25$ and $p \approx 1.2$, $(b/l \approx 0.12, kb \approx 1.11)$ above which increasing the value of kl lowers the efficiency substantially, in contrast with the RFT results. In the kl view (Figure 32b) it can be seen that the most efficient sine for each kl value occurs in lower amplitudes as kl grows. The kb value is changing from $kb \sim 1$ for low kl to $kb \sim 1.3$ for high kl, as in the infinite filament. The same results are plotted together as a function of kb in Figure 33. The solid line is the RFT prediction of the efficiency for an infinite swimmer with force ratio of $\xi = 1.51$. The filled red triangle display the efficiency of the best performing distance–wise sine wave. There is a good agreement between the RFT and the particle-based calculations for high p values and low kb values. As before, when kb increases the RFT overestimates the swimming efficiency.

The best swimming gait based on distance covered in a period has somewhat low efficiency of 1.7% with parameters: $kl \approx 8.86$, $b/l \approx 0.24$ and $D/l \approx 0.1167$. At a very low cost in the distance we can find a more efficient sine wave with parameters: $kl \approx 9.25$, $b/l \approx 0.2$ and $D/l \approx 0.1154$, which has efficiency of $\approx 2\%$. On the other hand, the most efficient swimmer performs quite well in terms of swimming distance, as $D/l \approx 0.093$. Therefore, keeping the undulation amplitude b/l in the range $0.12 \leq b/l \leq 0.24$ at the fixed wavelength $kl \sim 9.2$ would yield good swimming performance both speed-wise and power-wise.



Figure 32: Hydrodynamic efficiency, δ vs. bl, in the particle-based calculation. (a) In lines of equal p; (b) in lines of equal kl. The solid lines connect the markers for better view.



Figure 33: Hydrodynamic efficiency, δ , vs. kb. Comparison of particle-based computation results for several values of kl and p as in Figure 32, vs. the RFT prediction (3.11) for an infinite or unidirectional swimmer with $\xi = 1.51$ (thick solid line); the filled triangle (\triangleright) stands for the efficiency of the best performing distance-wise sinusoidal waveform.

Further insight of the locations of distance and efficiency maxima in the kl, b/l landscape can be gained using contour plots. The RFT method is less costly in terms of computer-time compared to the particle-based calculation, thus enables the calculation of smooth contours as displayed in Figure 34. Figure 34a depicts the contour graph of D/l as a function of kl and b/l, and Figure 34b depicts the efficiency in the same manner. The red dashed lines are equal p lines as in Figure 25, and the black dashed line present the limit of RFT validity. As explained before, the formal limit is $\kappa a \propto 1$, where κ is the local curvature of the filament, that can be re-written as $kb(kl) \propto 2\epsilon^{-1}$. From the results shown in Figure 24, the more accurate limit was found to be $kb(kl) = 0.5\epsilon^{-1}$. Above this limit the RFT overestimates the distance and the efficiency as seen in Figure 30 and Figure 33. The blue diamond marks the maximum distance swimmer in the particle-based computation, and the red star marks the most efficient one. It can be seen that the maximum of RFT distance per stroke is quite close to the particle-based one. This is different when the efficiency is concerned, as the efficiency in RFT gets higher as kl grows while the particle-based global maximum is in relatively low kl. The black solid lines in Figure 34a and b corresponds to $kb \approx 1.15$ and $kb \approx 1.3$ which are the kb values maximizing the distance and efficiency in the case of an infinite swimmer, based on equations (3.1) and (3.11) respectively. It can be seen that for the efficiency, the curve fitting the infinite swimmer crosses inside the white region of maximum efficiency for the final filament, while for the distance this is not the case. Figure 34c shows the contours of hydrodynamic efficiency δ in black on top of contours of scaled distance per stroke, D/l in blue. It shows that there is a large region in which both the distance and the efficiency are close to their maxima. This region, of $kl \approx 8-12$ and $b/l \approx 0.1-0.3$, should be a fine compromise for swimmers trying to optimize both parameters.





Figure 34: Color contour plots based on prediction of local RFT for a filament of the aspect ratio $\epsilon = 1/30$ in plane of parameters (b/l, kl). The corresponding sections of fixed mean p are shown as thin dashed lines (red, short dashes). The thick dashed line (black, long dashes) stands for the boundary of formal validity of the RFT, i.e. $kb(kl) = 0.5\epsilon^{-1}$. The filled symbols \blacklozenge and \star mark the parameters of the best gaits, distance-wise and efficiency-wise, respectively, determined particle-based in computations; (a) scaled distance per period of undulation D/l, the thick solid line stands for the location of the maximum velocity for an infinite filament based on Eq. (3.1), i.e. $kb \approx 1.15$; (b) hydrodynamic efficiency δ ; the thick solid line stands for the location of the optimal δ for an infinite filament based on Eq. (3.11), i.e. $kb \approx 1.3$; (c) Contours of hydrodynamic efficiency δ in black on top of contours of scaled distance per period of undulation, D/l in blue.

Figure 35 depicts the influence of the slenderness of the filament on the RFT prediction for the contours of D/l and δ . The dependency is expected to be weak, since the only parameter affected by it in the RFT calculation is $\xi = f_{\perp} / f_{\parallel}$, and it is a weak (logarithmic) function of ϵ ; the value of ξ increases from ~1.4 to ~1.7 as ϵ decreases from 1/12 to 1/800 -- by nearly 60 folds. Figure 35a shows the contours for the distance per stroke, dashed red for $\epsilon = 1/12$ and solid black for $\epsilon = 1/800$. The contours of the efficiency are presented in Figure 35b in the same manner. It can be readily seen that the variance in ξ has only a minor effect on the location of the optima for both D/l and δ . The long dashed red line marks the limit of validity of the RFT results for $\epsilon \approx 1/12$. The limit of validity for $\epsilon \approx 1/800$ has the value of $kb(kl) \approx 400$ which is beyond the limits of this figure axes range. The maximum distance $D/l \approx 0.101$ is achieved at $kl \approx 9.75$ and $b/l \approx 0.28$ for $\xi = 1.4$ and $D/l \approx 0.159$ at $kl \approx 8.75$, $b/l \approx 0.32$ for $\xi = 1.7$; the peak efficiency achieved at the maximal plotted kl = 12.5 (higher kl will yield slightly higher efficiency) is for $b/l \approx 0.1$ and has the values of $\delta \sim 2.2\%$ and $\sim 4.9\%$ for $\xi = 1.4$ and $\xi = 1.7$, respectively.



Figure 35: The effect of the filament slenderness on the swimming performance as predicted by the RFT in plane of parameters kl and b/l; dashed (red) curves stand for filament with aspect ratio $\epsilon \approx 1/12$ ($\xi = 1.4$), solid (black) lines correspond to the filament with $\epsilon \approx 1/800$ ($\xi = 1.7$). The long dashed red line marks the limit of validity of the RFT results for $\epsilon \approx 1/12$. The limit for $\epsilon \approx 1/800$ is beyond the limits of the figure. (a) Contours of the swimming distance per stroke, D/l; (b) Contours of swimming efficiency δ .

3.3.3 Changing the distance between spheres

To understand the significance of the internal structure of the swimmer on the results of the particle-based simulations, swimmers with different distance between the spheres were considered. First we calculated the drag coefficients f_{\perp} , f_{\parallel} and their ratio ξ for rods built from spheres with different aspect ratios, with the distance between spheres changing from d=2.02 to d=16. The results are displayed in Figure 36. The calculations were done as in section 3.2.4. For each calculation a straight rod built from N_p spheres was given a velocity in the perpendicular or tangent directions, and the resulting hydrodynamic force on it was calculated. Figure 36a shows the results for the calculations of ξ as a function of the aspect ratio for different distances between the spheres (squares). The results were fitted to the model function suggested before,

 $\xi \approx c_1 \left(\frac{1 - c_2 E}{1 + c_2 E} \right)$ (section 3.2.4), where $E = (\ln 2 / \epsilon)^{-1}$, and the parameters of the fit are presented in Table 1. For all the distances between spheres calculated, the fit of the results to the function

was very good (>98%).



Figure 36: (a) calculations of ξ as a function of the aspect ratio for different distances between the spheres (squares). The solid lines are a fit to the model function $\xi \approx c_1 (1-c_2 E)/(1+c_2 E)$, with the parameters as presented in Table 1. (b) The force coefficients as a function of the aspect ratio for rods with different distances between the spheres.

Figure 36b displays the coefficients calculated for different rods. It can be seen that as the distance between the spheres increases, both coefficients has lower value (meaning it is easier to move the rod), however the f_{\perp} coefficient is more affected than f_{\parallel} .

d	2.02	3	5	8	16
C_1	1.985	1.946	1.854	1.710	1.471
<i>C</i> ₂	0.523	0.545	0.616	0.648	0.587
The function $(1 - E)/(1 - E)$					

Table 1: Parameters of the fit to the model $\xi \approx c_1 (1 - c_2 E) / (1 + c_2 E)$



Figure 37: Calculation results for swimmers undulating in a sine wave with the parameters kl = 6, b/l = 0.216, length l = 62, and distances between spheres 2.07, 3 and 4. (a) Path in the XY plane. (b) Dissipation rate as a function of time.

The swimming of three swimmers with the same length l = 62 and different distance between spheres is compares in Figure 37. The undulation function for the swimmers was a sine wave with the parameters kl = 6, b/l = 0.216. The distance between spheres was 2.07, 3 and 4, and the number of spheres was 30, 21 and 16 respectively. As expected, the swimming distance reduces as the distance between spheres increases, since the force asymmetry, which is the driving force of the swimming of slender filaments in low Reynolds number, is lower. As can be seen in Figure 37b, increasing the distance between spheres also reduces the dissipation rate, however, the decrees is not very significant. This mild decrees shows that the dissipation component resulting from tight flow between the spheres is small.

3.3.4 Biological swimmers

To address the biological relevance of our results, we have collected from the literature values of kl, b/l and D/l for common undulatory biological swimmers such as sperm cells and nematodes, and compared them with our sinusoidal swimmer, in Figure 38 and Figure 39. The squares (\Box) correspond to the data for sperm cells, the circles (\circ) stand for various nematodes and the upper triangle is a flagellate [66]. Values of efficiency are not commonly calculated / measured for biological swimmers, so we could not compare them, except for our calculation of the efficiency of *C. elegans* brought in the following section. Figure 38 shows the parameters of the swimmers together with the parameters for the best sine waves efficiency-wise and distancewise; on top of the RFT contour plots of the distance (a) and efficiency (b). It is important to emphasize that the symbols for the different swimmers are located in Figure 38 according to the values of kl and b/l of their swimming stroke, but their distance per stroke value is typically higher than the value of the RFT contours in the same location. However, it can be seen that despite the fact that the swimmers employ undulations which are different from a sine wave, the swimming parameters of most of them are quite close to the maxima of efficiency and distance of the finite swimmer.



Figure 38: The comparison of parameters of undulating microorganisms (empty symbols) vs. a best-performing distance-wise (\bigstar) and efficiency-wise (\bigstar) filament with aspect ratio $\epsilon = 1/30$ propelled by a plain sinusoidal waveform determined by particle-based simulations, on top of the RFT contour plots as in Figure 34. The squares (\Box) correspond to the data for sperm cells (*P. miliaris* [64]; bos, chaetopterus, ciona, colobopocentotrus, lytechinus, psammechimus [63]; ostrea, ovis [65]), the circles (\circ) stand for the data for nematodes (*C. elegans* [60]; Haemonchus contortus, Turbatrix aceti, Pamagrellus silusia [66]); (a) On contours of D/l vs. scaled wave number kl and scaled amplitude D/l: (b) On contours of efficiency vs. scaled wave number kl and scaled amplitude b/l.

Figure 39 depicts the scaled distance per stroke for the biological swimmers and the best sine waves as a function of the wave number kl. Both sine waves are in the middle of the sperm cells group, and below the nematodes group which are performing better distance–wise (and also in the efficiency as we shall see in the following).



Figure 39: D/l vs. scaled wave number kl for undulating microorganisms (empty symbols) vs. a best-performing distance-wise (\blacklozenge) and efficiency-wise (\bigstar) filament with aspect ratio $\epsilon = 1/30$ propelled by a plain sinusoidal waveform determined by particle-based simulations. The squares (\Box) correspond to the data for sperm cells (*P. miliaris* [67]; bos, chaetopterus, ciona, colobopocentotrus, lytechinus, psammechimus [66]; ostrea, ovis [68]), the circles (\circ) stand for the data for nematodes (*C. elegans* [63]; Haemonchus contortus, Turbatrix aceti, Pamagrellus silusia [69]) and the upper triangle (Δ) is an eukaryote flagellate (Ochromonos malhamensis [66]).

3.3.5 <u>Nematode C. elegans</u>

The particle-based algorithm enables calculation of the swimming for any deformation function provided, assuming the locations of the spheres are continuous. It uses a vector of locations in times, $\mathbf{X} = \{(x_{ij}, y_{ij}, z_{ij})\}$ for $i = 1...N_p$, $j = 1...N_t$, where N_p is the number of spheres and N_t the number of time steps. Thus it enables us to calculate the swimming due to the experimental deformation function of *C. elegans*.

The swimming gait adopted in computation was extracted from videos shot with a highspeed camera via the use of custom-written image processing algorithm [62]. The snapshots of the nematode waveforms (in the co-rotating and co-moving frame) are shown in Figure 40, compared with a sine wave with the parameters kl = 9, b/l = 0.2, p = 0.8, in the geometrical center frame of reference. As can be seen, the deformation function of the nematode is quite different from a sine wave, the main difference being significant variation in the amplitude along the body. The deformation function can be divided to three parts, the head and tail which undulate in a relatively high amplitude, and the middle part which undulates with lower amplitude. Between these parts there are two zones with significantly low amplitude. The nematode in the figure is propelled to the right, and it is noticeable that despite the relative symmetry between the head and tail, the head part moves with higher curvature.

To simulate the typical aspect ratio of the nematode, of $\epsilon = 0.083$ (typical length of ~1mm and width of ~0.08mm), we used a swimmer made of 12 spheres, and the swimming was calculated in the same way as for the sine wave swimmers, as well as the calculation of the power and efficiency of the stroke. As depicted in Figure 41, there is a very good agreement between the experimentally probed trajectory and the numerically calculated path using the tabulated deformation shown in Figure 40. This agreement justifies the use of low Reynolds hydrodynamics in *C. elegans* locomotion study whereas typically $Re \sim 1$ in low viscosity aqueous medium. The typical parameters for *C. elegans* propulsion are $b/l \approx 0.12$, $kl \approx 7.9$ and $D/l \approx 0.17$ as reported in [62]. The calculated efficiency has an unexpectedly high values of ~ 8.8%, which is even higher than the optimal swimming efficiency corresponding to Lighthill's sawtooth traveling wave propagating along infinite filament which is $\delta = 8.58\%$ [32]. The





Figure 40: (a) The snapshots of the nematode waveforms in the co-rotated and co-moving frame of reference as tracked in the experiment in [62]; the worm is propelled head to the right. (b) The deformation function of a sine wave with the parameters kl = 9, b/l = 0.2, p = 0.8, in the geometrical center frame of reference.

Even though the nematode does not use a simple sine wave, the parameters of the sine waveform optimized to the furthest advancement per stroke are similar to the values employed by the nematode (see the comparison in Figure 38). However, the shape of the waveform exploited by the worm allows a considerably superior locomotion (in terms of both the displacement per stroke and efficiency!) compared with the sine waveform optimized for the furthest displacement showing $D/l \approx 0.12$ and $\delta \approx 2$. One significant difference is that the nematode does very little rotation during the stroke; the maximum pitching angle is $\theta_m \approx 6^\circ$, compared with $\theta_m \approx 53^\circ$ for the sine wave advancing the maximum distance per stroke, and similar to the efficient sine wave for which $\theta_m \approx 9.5^\circ$.

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Figure 41: The trajectory of the geometric center of the nematode: tracking experiment (Red line) and particle-based simulation (Blue line). The worm in this experiment was ~1.2mm long, and it progressed ~0.2mm per period of undulation, yielding $D/l \approx 0.17$.

3.4 Conclusions

This work began with two main questions in mind: the first was what is the best finite sinusoidal swimmer and whether its parameters comply with the predictions of an infinite sinusoidal swimmer, and the second concerned the specific swimming gait of the nematode *C*. *elegans* and its optimality.

To answer these questions we calculated the advancement, pitching and dissipation for a sinusoidal swimmer with wide range of wave numbers and amplitudes, employing two computation methods, namely particle-based algorithm and RFT. The comparison between the methods revealed that the inter-filament hydrodynamic interactions become important when $kb(kl) \approx 0.5\epsilon^{-1}$, above which the RFT overestimates the advancement of the swimmer and its efficiency. Comparing to the infinite swimmer, the finite sinusoidal swimmer has global maximum of distance per stroke at the parameters $p \approx 0.8$, $b/l \approx 0.24$, and $kl \approx 8.86$, for which $D/l \approx 0.1167$. These parameters are distant from the line of kb = 1.15 yielding the maximum velocity for the infinite swimmer. The efficiency maximum, on the other hand, is located close to the line of $kb \approx 1.29$ appropriate for the maximum efficiency for the infinite swimmer. For the finite swimmer, however, there is a global maximum of $\delta \approx 2.8\%$ around relatively low values of $kl \approx 9.25$ and $p \approx 1.2$, $(b/l \approx 0.12, kb \approx 1.11)$ and the high kl global maximum is correct only for very slender filaments. Comparing contours of distance per stroke and efficiency, we found a large region in the parameters space in which both the distance and the efficiency are close to their maxima. This region, of $kl \approx 8-12$ and $b/l \approx 0.1-0.3$, should be a fine compromise for swimmers trying to optimize both parameters. Available data for undulatory micro-swimmers including various sperm cells and nematodes shows that despite the difference between their deformation function and a sine wave, most of them operate in a narrow range of wavelengths and amplitudes $kl \approx 7.5 - 11.5$, $b/l \approx 0.08 - 0.16$, which is similar to the preferred region found for the sine waves swimmers.

Concentrating on *C. elegans*, we calculated its swimming from its experimental deformation function, using the particle-based algorithm, and reached a good agreement with the experimental path of the geometrical center. This verifies the use of low Re calculations for the simulation of *C. elegans* swimming which in water has Re~1. From this calculation the distance

per stroke and the efficiency of the nematode swimming were extracted, both revealed to be much higher than the sine waves displacement and efficiencies. This demonstrates the superiority of the nematode swimming stroke, presumably achieved by employing significant amplitude changes between different parts of its body.

A straightforward extension of this work would be to explore deformation functions with features resembling the *C. elegans* swimming stroke. The thorough parametric mapping of efficiency and distance per stroke which was done for the sine wave can be repeated for deformation functions with significant amplitude modulation along the swimmer's body. The location of the nematode's experimental parameters on such mapping would indicate the objective function which the nematode optimizes, which presumably would be some compromise between efficiency and speed. Also, the swimming of sperm cells can be simulated using the particle-based algorithm which allows the simulation of a swimming filament carrying a large head.

4 Appendix

4.1 <u>Particle-based computation scheme</u>

The general solution for the velocity field around a collection of N_p spherical particles of radii a_i , can be written in terms of solid spherical harmonics as $\mathbf{v}^0 = \sum_{j=1}^{N_p} V_j$, where the solution outside a single ith sphere has the form of Lamb's general solution of Stokes equations [64]:

(4.1)
$$V_{j} = \sum_{n=1}^{\infty} \nabla \times \left(r_{j} \chi_{-(n+1)}^{j} \right) + \nabla \phi_{-(n+1)}^{j} - \frac{(n-2)}{2n(2n-1)} r_{j}^{2} \nabla p_{-(n+1)}^{j} + \frac{(n+1)}{n(2n-1)} r_{j} p_{-(n+1)}^{j}$$

Here \mathbf{r}_i is the radius vector with origin at the center of the ith sphere, $r_i = |\mathbf{r}_i| = a_i$, $\chi^i_{-(n+1)}$, $\Phi^i_{-(n+1)}$ and $p^i_{-(n+1)}$ are the linear combinations of solid harmonics u^i_{mn} with the origin at the center of the ith sphere,

m = -n

(4.2)

$$\Phi_{-(n+1)}^{j} = \sum_{m=-n}^{n} a_{mn}^{j} u_{mn}^{j-}$$

$$p_{-(n+1)}^{j} = \sum_{m=-n}^{n} b_{mn}^{j} u_{mn}^{j-}$$

$$\chi_{-(n+1)}^{j} = \sum_{m=-n}^{n} c_{mn}^{j} u_{mn}^{j-}$$

(4.3)
$$u_{mm}^{j-} = \frac{1}{r^{n+1}} P_n^m \left(\cos \theta_j \right) e^{im\phi_j}$$

where P_n^m is the associated Legendre function. The no-slip boundary conditions, $\mathbf{v} = \mathbf{u}_i$, where \mathbf{u}_i is the local velocity of the surface of ith particle, can be used to determine the unknown coefficients a_{mn}^i , b_{mn}^i and c_{mn}^i . An elegant way of computing the coefficients was proposed in [59]. The boundary conditions are first transformed to the Lamb's form by applying operators $\mathbf{r}_i \cdot$, $-r_i \nabla \cdot$ and $\mathbf{r}_i \cdot \nabla \times$ to both sides of the no-slip boundary condition and then the direct origin-toorigin transformation of spherical harmonics centered at different spheres is applied, yielding an infinite system of linear equations for the coefficients,

$$(4.4) \qquad -(n+1)a_{mn}^{i} + \frac{(n+1)}{2(2n-1)}b_{mn}^{i} + a_{i}^{2n+1}\sum_{j=1}^{N}\sum_{l=1}^{\infty}\sum_{k=-l}^{l}\left(D_{klmn}^{ij}a_{kl}^{j} + E_{klmn}^{ij}b_{kl}^{j} + F_{klmn}^{ij}c_{kl}^{j}\right) = a_{i}^{n+1}X_{mn}^{i},$$

$$(4.4) \qquad \frac{1}{a_{i}^{2}}(n+1)(n+2)a_{mn}^{i} - \frac{n(n+1)}{2(2n-1)}b_{mn}^{i} + \sum_{j=1}^{N}\sum_{l=1}^{\infty}\sum_{k=-l}^{l}\left(G_{klmn}^{ij}a_{kl}^{j} + H_{klmn}^{ij}b_{kl}^{j} + L_{klmn}^{ij}c_{kl}^{j}\right) = a_{i}^{n}Y_{mn}^{i},$$

$$n(n+1)c_{mn}^{i} + a_{i}^{2n+2}\sum_{j=1}^{N}\sum_{k=-l}^{\infty}\left(M_{klmn}^{ij}b_{kl}^{j} + N_{klmn}^{ij}c_{kl}^{j}\right) = a_{i}^{n+1}Z_{mn}^{i}.$$

The coefficients $D_{mnkl}^{ij}, E_{mnkl}^{ij}, F_{mnkl}^{ij}, K_{mnkl}^{ij}, L_{mnkl}^{ij}, M_{mnkl}^{ij}$ and N_{mnkl}^{ij} are given in the appendix of [59] in terms of the transformation coefficient C_{klmn}^{ij} :

$$C_{klmn}^{ij} = (-1)^{m+n} \frac{(l+n-k+m)!}{(l-k)!(m+n)!} u_{(k-m)(l+n)}^{j-}(R_{ij},\theta_{ij},\varphi_{ij}),$$

Where $R_{ij}, \theta_{ij}, \varphi_{ij}$ are the coordinates of vector \mathbf{R}_{ij} connecting the centers of jth and ith spheres in the spherical coordinate system centered at particle j, $u_{(k-m)(l+n)}^{j-}$ is the decaying spherical harmonic defined in (4.3). According to definition of spherical harmonics the coefficients C_{klmn} are assumed zero if |k| > l or if |m| > n.

 X_{mn}^{i} , Y_{mn}^{i} and Z_{mn}^{i} are the coefficients in the expansions in surface harmonics of $\frac{\mathbf{r}_{i}}{r_{i}} \cdot \mathbf{u}_{i}$, $-r_{i} \nabla \cdot \mathbf{u}_{i}$, $\mathbf{r}_{i} \cdot \nabla \times \mathbf{u}_{i}$. When the particle surface velocity corresponds to the rigid body motion, $\mathbf{u}^{i} = \mathbf{U}_{i} + \mathbf{\omega}_{i} \times \mathbf{r}_{i}$, the right hand side of (4.4) can be written as [59]:

$$X_{1n}^{i} = \frac{1}{2} \left(U_{ix}^{0} - i U_{iy}^{0} \right) \delta_{n}^{1} \qquad X_{0n}^{i} = U_{iz}^{0} \delta_{n}^{1} \qquad X_{-1n}^{i} = - \left(U_{ix}^{0} + i U_{iy}^{0} \right) \delta_{n}^{1}$$

$$(4.5) \qquad Y_{mn}^{i} = 0$$

$$Z_{1n}^{i} = \left(\omega_{ix}^{0} - i \omega_{iy}^{0} \right) \delta_{n}^{1} \qquad Z_{0n}^{i} = 2 \omega_{iz}^{0} \delta_{n}^{1} \qquad Z_{-1n}^{i} = -2 \left(\omega_{ix}^{0} + i \omega_{iy}^{0} \right) \delta_{n}^{1}$$

With $\{\mathbf{U}_i, \omega_i\}$ being the translation and rotation velocities of ith sphere, respectively and δ_n^k being the Kronecker's delta.

The viscous drag force \mathbf{F}_i exerted on sphere *j* and hydrodynamic torque \mathbf{T}_i about its center can be expressed in terms of the expansion coefficients,

(4.6)

$$F_{i} = -4\pi \left[\left(b_{11}^{i} - \frac{1}{2} b_{-11}^{i} \right) x + i \left(b_{11}^{i} + \frac{1}{2} b_{-11}^{i} \right) y + b_{01}^{i} \hat{z} \right]$$

$$T_{i} = -8\pi \left[\left(c_{11}^{i} - \frac{1}{2} c_{-11}^{i} \right) x + i \left(c_{11}^{i} + \frac{1}{2} c_{-11}^{i} \right) y + c_{01}^{i} \hat{z} \right]$$

Thus when velocities of N_p spheres are prescribed the forces and torques exerted on any sphere can be found by solving $3N_p \times \mathcal{L} \times (\mathcal{L}+2)$ equations for the expansion coefficients $\{a_{nm}^i, b_{nm}^i, c_{nm}^i\}$, obtained by truncating the series in Eqs (4.4) after \mathcal{L} terms, together with using (4.6). Alternatively, forces and torques can be prescribed and velocities are computed or a mixed problem can be formulated when some velocities and forces/torques are prescribed
4.2 <u>Parameterization and incompressibility constraint in the RFT</u>

This section details additional subjects concerning the derivation of RFT for the finite swimmer in plane motion brought in 3.2.3.1.

In our description of the swimmer as $\mathbf{r}_0(s,t)$, we parameterized it using a parameter *s*. It was implicitly assumed that each specific value of *s* corresponds to specific material point of the swimmer. i.e. a specific material point at $\mathbf{r}_0(s,t_2)$ at time t_2 is the same one which was at $\mathbf{r}_0(s,t_1)$ at time t_1 . If this assumption fails, then the calculation described above would fail too. In most biological cases the filament is assumed to be incompressible. This automatically implies that a good parameterization corresponding to actual material points is by its proper length parameter. In such case the correct parameterization should be through the proper length $\zeta = \int \gamma ds = \int \left| \frac{\partial \mathbf{r}_0}{\partial s} \right| ds$ rather than by *s*. The above formulation would still hold provided we interpret $\mathbf{v}_0 \equiv \dot{\mathbf{r}}_0$ as a derivative at constant proper length ζ rather than at constant *s*,

(4.7)
$$\mathbf{v}_{\mathbf{0}} = \dot{\mathbf{r}}_{\mathbf{0}} = \left(\frac{\partial \mathbf{r}_{\mathbf{0}}}{\partial t}\right)_{\zeta} = \left(\frac{\partial \mathbf{r}_{\mathbf{0}}}{\partial t}\right)_{s} + \left(\frac{\partial \mathbf{r}_{\mathbf{0}}}{\partial s}\right)_{t} \left(\frac{\partial s}{\partial t}\right)_{\zeta}.$$

Actual implementation of this requires calculating $(\partial s / \partial t)_{\zeta}$ as a function of (s, t) for the prescribed undulating filament.

Alternatively, the velocity in (4.7) can be expressed as

(4.8)
$$\mathbf{v}_{0} = \frac{\partial \mathbf{r}_{0}}{\partial t} + \alpha(s, t)\hat{\mathbf{s}}$$

for some $\alpha(s,t)$ where $\hat{\mathbf{s}} = \gamma^{-1} \frac{\partial \mathbf{r}_0}{\partial s}$ is the local unit tangent. In other words, the second term on the r.h.s. of Eq. (4.7) can be interpreted as an extra tangential velocity. Demanding incompressibility requires vanishing of the 1D velocity divergence $\nabla_s \cdot \mathbf{v}_0 = \hat{\mathbf{s}} \cdot \frac{\partial \mathbf{v}_0}{\partial s} = 0$. Solving

this equation we find $\alpha(s,t) = -\int \hat{\mathbf{s}} \cdot \frac{\partial^2 \mathbf{r_0}}{\partial s \partial t} ds + C(t)$ up to some arbitrary function of time C(t).

The integration constant C(t) may be determined by considering the boundary conditions at the swimmer edges. Note that if s is not proportional to the proper length parameter ζ then incompressibility constraint also implies that its range $s \in [s_0, s_1]$ must be time-dependent, $s_0 = s_0(t), s_1 = s_1(t)$. The constraint $l = \int_{s_0}^{s_1} \gamma ds$ does not determine the endpoint s_0, s_1 uniquely. Only by specifying an extra condition (e.g. requiring s_0 or s_1 or their average to vanish) does one completely define the swimming mode. The possible arbitrariness of $s_0(t)$ does not matter however, in the special case of our main interest where $\mathbf{r}_0(s,t)$ corresponds to the traveling wave $\mathbf{r}_0 = \{s, \phi(ks - \Omega t)\}$. Indeed any choice of (periodic) $s_0(t)$ may be compensated by redefining the $t' = (\Omega t - ks_0(t)) / \Omega$ (and applying the time parameter as 'gauge' transformation $\mathbf{R}(t) \rightarrow \mathbf{R}(t) - \hat{x}s_0(t)$). Thus in the following we use the simplest choice namely $s_0(t) = 0$. Since the velocity of the endpoint (which is a material point) at $s = s_0$ is $\mathbf{v}_0 = \frac{\partial \mathbf{r}_0}{\partial t} + \frac{\partial \mathbf{r}_0}{\partial s} \frac{ds_0}{dt}$ we see that the condition $s_0 \equiv 0$ imply $\alpha|_{s=0} = 0$ and hence $\alpha(s,t) = -\int_0^s \hat{s} \cdot \frac{\partial^2 \mathbf{r}_0}{\partial s \partial t} ds$. For the specific example

 $\mathbf{r}_0(s,t) = \{s, b \sin(ks - \Omega t)\}$ we obtain

(4.9)
$$\alpha(s,t) = \frac{\Omega}{k} \left[\sqrt{1 + (kb)^2 \cos^2(ks - \Omega t)} - \sqrt{1 + (kb)^2 \cos^2(\Omega t)} \right].$$

The equation $l = \int_0^{s_1} \gamma ds$ determining $s_1(t)$ leads in the case of the sine wave to

(4.10)
$$\frac{kl}{\sqrt{1+(kb)^2}} = E\left(\Omega t, \frac{(kb)^2}{1+(kb)^2}\right) - E\left(\Omega t - ks_1(t), \frac{(kb)^2}{1+(kb)^2}\right)$$

where $E(\varphi, m) = \int_0^{\varphi} (1 - m \sin^2 \theta)^{1/2} d\theta$ is the elliptic integral of the second kind. Only in the special case where the sine wave contains exactly half integer number p of periods, one finds that $s_1(t) = p\pi/k$ becomes t-independent. In this special case one may relate k and p as $\frac{1}{kb}E(-(kb)^2) = \frac{l}{4bp}$, where $E(m) = E(\pi/2, m)$ is a complete elliptic integral.

4.3 Useful identities

Denoting
$$\langle ... \rangle = \frac{1}{\lambda} \int_0^{\lambda} (...) ds$$
, for $\gamma = \frac{d\zeta}{ds} = (\hat{\mathbf{s}} \cdot \mathbf{x})^{-1} = \sqrt{1 + (kb)^2 \cos^2(ks - \Omega t)}$ we have:
 $\langle \gamma \rangle = \frac{2}{\pi} E(-(kb)^2),$
 $\langle \frac{1}{\gamma} \rangle = \frac{2}{\pi} K(-(kb)^2),$
 $\langle \gamma^2 \rangle = 1 + (kb)^2 / 2,$
 $\langle \frac{1}{\gamma^2} \rangle = \frac{1}{2\sqrt{1 + (kb)^2}}.$

5 <u>References</u>

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קרוב ל-1. בנוסף למסלול המרכז הגאומטרי, חישבנו באלגוריתם מבוסס החלקיקים את מרחק ההתקדמות של הנמטודה ויעילות השחיה שלה, ושניהם התקבלו גבוהים משמעותית מהתוצאות האופטימליות של גלי הסינוס שנידונו קודם לכן. זוהי הדגמה לכך שצורת החבטה של הנמטודה, אשר מאפיין מרכזי בה הוא שינויים משמעותיים באמפליטודה לאורך גוף השחיין, עדיפה על גל סינוס פשוט. התקדמות השחיינים חושבה בעזרת שתי שיטות. הראשונה היא חישוב בעזרת אלגוריתם נומרי מבוסס חלקיקים, בו השחיין נבנה ממערך של כדורים, ושדה הזרימה מסביב לכדורים נפתר באופן מדויק. השיטה השניה היא (Resistance Force Theory (RFT, ובה מזניחים את האינטראקציות ההידרודינמיות בין חלקים שונים של השחיין. ההנחה היא שהשחיין דק מספיק, כך שהכוח על כל אלמנט אורך ניתן לביטוי בעזרת רכיב המהירות המקביל והניצב לאלמנט האורך, עם מקדמי פרופורציה קבועים. היתרון של שיטה זו שהיא מאפשרת חישובים נומריים מהירים ופיתוחים אנליטיים.

ההשוואה בין שיטות החישוב אפשרה למצוא את גבול התקפות של RFT, מעליו ההזנחה של האינטראקציות ההידרודינמיות פוגעת באופן משמעותי בדיוק התוצאות. מעבר לגבול זה ערכי היעילות ומרחק ההתקדמות המתקבלים מ RFT הם בעלי ערכים גבוהים מדי. גבול זה נקבע על ידי דקיקות השחיין ביחס לעקמומיות המקומית של פונקציית הדפורמציה.

עבור שחיין אינסופי, ישנו קו במרחב הפרמטרים של מספר גל ואמפליטודה עליו מתקבלת ההתקדמות המקסימלית, וקו דומה עבור היעילות המקסימלית. לעומת זאת, עבור שחיין סופי מצאנו מקסימות גלובליות עבור גדלים אלו בערכים נמוכים של מספר הגל, ומקסימום המרחק בחבטה עבור שחיין סופי נמצא רחוק מהקו המאפיין את השחיין האינסופי. בדומה לעבודות קודמות, בחישוב בשיטת RFT קיבלנו כי קיימות מקסימות מקומיות של יעילות בערכי מספר גל נמוכים יחסית, אולם המקסימום הגלובלי הוא במספרי גל גבוהים ככל האפשר, בדומה לשחיין אינסופי. לעומת זאת, חישוב באמצעות אלגוריתם מבוסס חלקיקים הראה כי לשחיין שאינו מאד דק מתקבל מקסימום גלובלי בערכי מספר גל נמוכים. מקסימום זה נמצא קרוב לקו המאפיין את היעילות המקסימלית של השחיין האינסופי.

החישובים בשיטת RFT אפשרו לנו לחשב קונטורים של יעילות ומרחק שחיה בחבטה. מצאנו כי קיים אזור במרחב הפרמטרים של מספר הגל ואמפליטודת הגל בו גם יעילות השחיה וגם המרחק בחבטה גבוהים. זהו אזור פרמטרים מוצלח לשחיינים המעונינים באופטימליות של שני המדדים גם יחד. השוואה לשחיינים ביולוגיים העלתה כי הם פועלים בתחום פרמטרים שני, הקרוב לתחום הפרמטרים המתאים לגל הסינוס. זאת למרות ההבדלים בין צורת החבטה שלהם וגל סינוס.

לבסוף, התמקדנו בנמטודה *C. elegans*. בעזרת האלגוריתם מבוסס החלקיקים, חישבנו את מסלול ההתקדמות של המרכז הגאומטרי של הנמטודה מתוך פונקצית הדפורמציה הניסיונית המדודה שלה, וקיבלנו התאמה טובה בין המסלול המדוד והמחושב של המרכז הגיאומטרי. התאמה זו מאשרת כי חישוב התנועה של הנמטודה באמצעות הידרודינמיקה של מספר ריינולדס נמוך הוא מדויק מספיק, למרות שמספר הריינולדס של שחיית *C. elegans* במים אינטראקציה זו לא נידונה בעבודות קודמות, ואנו מראים כי היא יכולה להביא להסתדרות של המקלות באותו כיוון, כתלות בתכונות המנוע המולקולרי. בדקנו מספר תכונות אפשריות של המנוע, ומצאנו כי תכונות מנוע היוצרות סדר הן התנתקות ספונטנית אקראית מהמקל, בשילוב עם מהירות התקדמות התלויה בזווית שבין המקלות או בשינוי הזווית שבין המקלות. מגע הנעה על שני מקלות בו זמנית. בניגוד לעבודות קודמות, במודל שלנו אינטראקציה זו מגע הנעה על שני מקלות בו זמנית. בניגוד לעבודות קודמות, במודל שלנו אינטראקציה זו היא סימטרית לגמרי ולא מביאה להתיישרות של המקלות ולכן אינה יכולה להביא לסדר. בנוסף לאינטראקציה בין זוגות, חישבנו את התנועה של מבנים מורכבים יותר. במבנה של משולש מקלות הנסגר על ידי מנוע מולקולרי, הראינו כי במשולש שאינו שווה צלעות צפויים כוחות גדולים מאד בזמן סגירת המשולש הגורמים למנוע להתנתק מהמקל ובכך להתפרקות המשולש. בעיה נוספת אותה פתרנו היא הבעיה של צורות משוכללות של מקלות המחוברים על ידי מנועים. הראינו כיצד צורות אלו נסגרות ליצירת כוכב של מקלות, ואת ההבדל בין תנועת מקלות בתווך בעל ריינולדס נמוך ובין תנועת מקלות ללא גרר.

החלק השני של העבודה עוסק בשחיה של חוט בעל אורך סופי בתווך בעל מספר ריינולדס נמוך. בתווך זה, המשוואות המתארות את התנועה הן משוואות סטוקס שהן לינאריות ולא תלויות בזמן. בשל כך, על מנת לשחות על השחיין לבצע סדרת תנועות מחזורית אך לא סימטרית בזמן. אחת האסטרטגיות של מיקרואורגניזמים היא שחיה באמצעות שינוי צורה מחזורי בצורת גל מתקדם של איבר חוטי כגון שוטון.

המוטיבציה לשאלת המחקר נובעת מהשחיה של הנמטודה C. elegans. זוהי תולעת שטוחה באורך של כ-1 מילימטר, החיה באדמה ומסוגלת לזחול בחומר גרגירי ולשחות בנוזל. התנועה של נמטודה זו נחקרה והתגלה כי היא מבצעת את אותה צורת שחייה בטווח רחב של תנאי צמיגות של התווך. נשאלת השאלה האם צורת שחייה זו אופטימלית במובן כלשהו מבחינת הנמטודה, או שהיא נובעת ממגבלות על מבנה השרירים או מערכת העצבים שלה. שאלה מתמטית כללית יותר הקשורה לכך היא שאלת השחייה האופטימלית עבור שחיין שהוא חוט סופי.

השאלה הספציפית אותה פתרנו היא שחיה של חוט סופי המתנודד בפונקציית דפורמציה של גל סינוס מתקדם. סקרנו את פרמטרי הגל בחיפוש אחר השחיין הטוב ביותר במדדים של יעילות שחייה ומרחק התקדמות בחבטה, המקובלים להשוואה בין שחיינים בתווך בעל מספר רינולדס נמוך. יעילות השחיה היא היחס בין האנרגיה המושקעת כדי לגרור שחיין פסיבי, לבין האנרגיה שאותו שחיין מוציא בשחיה של אותו מרחק. מדד זה מתאים כאשר לשחיין יש אנרגיה מוגבלת. מרחק מקסימלי בחבטה הוא אופטימיזציה גיאומטרית של צורת החבטה, ומתאים כאשר אין הגבלה על האנרגיה אלא על תדירות החבטות.

Ш

תקציר

בעבודה זו עסקנו בשתי שאלות מתוך התחום של הידרודינמיקה במספר רינולדס נמוך. מספר רינולדס הוא היחס בין רכיב התאוצה לרכיב הצמיגות בכוחות הפועלים על גוף הנע בתווך. במספר רינולדס נמוך, התנועה היא בעלת רכיב צמיגות משמעותי וללא תאוצה. תחום תנועה זה רלוונטי למשל למיקרואורגניזמים השוחים במים, ולתנועה של רכיבים מולקולריים בתוך תאים חיים. תופעות משני נושאים אלו נידונות בעבודה זאת, ונעשה עבורן מידול אנליטי ונומרי. החלק הראשון של העבודה נעשה בהשראת תופעת הסתדרות של מיקרוטובולים ומנועים מולקולריים, והוא עוסק בתנועה של מקלות המחוברים על ידי מנועים. החלק השני של העבודה מושפע משאלת השחייה של הנמטודה *C. Elegans* ועוסק בשחייה של חוט סופי המתקדם על ידי תנודה של גלי סינוס.

מיקרוטובולים הן מולקולות ארוכות העשויות מחלבונים ומהוות רכיב משמעותי במבנה תאים ביולוגיים. עבור מולקולות אלו, היחס בין האורך לרוחב קטן מ-0.001, ואורך ההתמדה (persistence length) שלהם הוא מספר מילימטרים, לכן ניתן למדל אותן בצורה טובה כמקלות קשיחים. אחד המנועים המתקדמים על מיקרוטובולים הוא המנוע המולקולרי קינסין, המשתמש במיקרוטובולים כמסילות ארוכות המאפשרות לו להוביל חומרים ממקום למקום בתא. מיקרוטובולים ומנועים מולקולריים משתתפים בתופעה מעניינת הנצפית בתאי ביצית של זבוב הפירות דרוזופילה. תופעה זו נקראת זרימה ציטופלסמית, ובה מתרחשת הסתדרות ספונטנית של מיקרוטובולים ממצב של רשת רנדומית למצב מסודר לאורך דפנות התא, ביחד עם ערבוב משמעותי של תוכן התא. הסתדרות ספונטנית דומה ניצפתה גם במערכות מהונדסות שהכילו מיקרוטובולים ומנועים מולקולריים בלבד. במערכות אלו, ההווצרות של צורות שונות כגון מערבולות וכוכבים היתה תלויה בריכוז המנועים המולקולריים במערכת. מידול תיאורטי של מערכות אלו נעשה בעבר על ידי ניתוחים אנליטיים וסימולציות, אולם ברובן הניחו השפעה חלשה של התווך ההידרודינמי על הסתדרות המערכת. ברוב המקרים, אכן כוח המנועים המולקולריים חזק בהרבה מהגרר שמפעיל התווך ההידרודינמי, אולם בתמיסות צפופות הצמיגות האפקטיבית עולה משמעותית ויכולה להביא לכוחות באותו סדר גודל של המנועים המולקולריים.

בהשראת בעיה זו, ניתחנו את האינטראקציה בין שני מקלות המחוברים על ידי מנועים מולקולריים. בשונה מעבודות קודמות אשר מידלו את המנועים המחוברים כקפיצים המקשרים בין שני המקלות, אנו מידלנו את המנועים כנקודות מגע קשיחות, המאפשרות סיבוב חופשי של המקלות סביבן. מודל זה מאפשר השפעה משמעותית יותר של כוח הצמיגות של התווך על תנועת המקלות. פתרנו את הבעיה עבור שתי אפשרויות חיבור של המנועים והמקלות. באפשרות הראשונה, מנוע אחד הולך על מקל ונושא מקל נוסף.

I

תודות

המחקר נעשה בהנחיית פרופ' יוסי אברון ופרופ' חבר אלכסנדר לישנסקי בפקולטה לפיסיקה.

ברצוני להודות למנחים שלי, פרופ' יוסי אברון ופרופ' חבר אלכסנדר לישנסקי. אלכס – תודה מקרב לב על העזרה, ההדרכה הזמן והמאמץ שהקדשת לעבודה הזו. יוסי – תודה על התמיכה, ההנחיה, והשאלות הקשות. להסביר לך תמיד דרש הבנה מעמיקה.

תודה לדר' עודד קנט על שיתוף הפעולה הפורה ותרומתו החשובה לעבודה, ולדר' ג'ושוע שניצמן על דיונים מעניינים ועל שיתוף ועזרה בעבודה עם המידע הנסיוני.

תודה למשפחתי: להורי, על עזרתם תמיד ובמיוחד בזמנים עמוסים, לילדי, שמזכירים לי מה חשוב בחיים, ולאיש שלי, על העזרה, הזמן, הסבלנות והעידוד כל השנים.

לליהוא,

שותפי בכל

ליהל ופלג,

מתנותי

שחייה וסדר בתווך צמיג

חיבור על מחקר

לשם מילוי חלקי של הדרישות לקבלת התואר דוקטור לפילוסופיה

רותם ש. ברמן

הוגש לסנט הטכניון – מכון טכנולוגי לישראל

חיפה

תמוז תשע"ג

יוני 2013

רותם ש. ברמן

שחייה וסדר בתווך צמיג