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SIMULATION OF PLANAR WAVE FLAGELLAR PROPULSION OF NANOROBOTS USING COMSOL

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Abstract: Advancement in the field of Nanorobotics has been facilitated by the current advances in Nano-bio-technology and nanofabrication techniques. Nanorobots can be used in the advancement of medical technology, healthcare and environment monitoring and swim in biological fluids flowing in narrow channels of a few hundred nanometers in the area of bio-medical engineering. The pronounced effects in nanometer scale such as increased apparent viscosity and low Reynolds number make the designing of propulsion mechanism a challenging task. Prominent modes of flagellar locomotion in micro-sized biological organisms are by generating planar waves or through helical rotation. The present work attempts to numerically simulate the shape form of the tail of a swimming nanorobot by solving the governing equation of its flagellar hydro-dynamics. It corroborates with the analytical studies aimed at the modeling of Nanorobot dynamics thorough planar wave propagation.

Keywords: Nanorobots, Planar Wave, Flagellar Hydrodynamics, Low Reynolds Number

1. Introduction

Advancement in the field of Nanorobotics has been facilitated by the current advances in Nano-bio-technology and nanofabrication techniques [1]. Development of nanorobots should facilitate medical technology, healthcare and environment monitoring. Bio-medical engineering research may develop nanorobtos that swim in biological fluids flowing in narrow channels of a few hundred nanometers for drug delivery or as probes. The pronounced effects in nanometer scale such as increased apparent viscosity and low Reynolds number make the designing of propulsion mechanism a challenging task [2]. Prominent modes of flagellar locomotion in micro-sized biological organisms are by generating planar waves or through helical rotation [3-6]. Efforts have been taken to mathematically model the same and implement it as the propulsion mechanisms for nanorobots. Out of the two popular modes, the present work attempts to numerically simulate the shape form of the tail of a swimming nanorobot executing planar wave propagation.

2. Mathematical Modeling

The governing equation of the swimming nanorobot is derived analyzing the flagellar hydro-dynamics. The robot system is divided into a head and a tail part where the propulsive force is generated by the tail. Assessing the tail configuration provides the boundary conditions.

Two sets of forces govern the motion of a flagellum. Namely elastic forces that tend to straighten the flagellum and viscous forces that oppose the motion of each element through the fluid medium. The two forces determine the form and rate of propagation of waves along flagella. Force balance is used to derive the resultant governing equation of motion; a fourth order partial differential equation (PDE) consisting of Young's modulus (E), Area moment of inertia (I), viscosity of the medium (μ) and Reynolds number (Re) terms (refer (1)).

$$EI(x)\frac{\partial^4 y}{\partial x^4} = -\frac{4\pi\mu}{2-\log(\text{Re})}\frac{\partial y}{\partial t} \quad (1)$$

For a spherical head attached to cylindrical tail the boundary conditions are as follows

At x=0

$$y = 0 \quad (2)$$

$$\frac{\partial y}{\partial x} = G\sin\omega t \quad (3)$$

where G is the amplitude of the planer wave

At x=L

$$\frac{\partial^2 y}{\partial x^2} = 0 \quad (4)$$

as bending moment vanishes at the end and

$$\frac{\partial^3 y}{\partial x^3} = 0 \quad (5)$$

as shear force vanishes at end

3. Use of COMSOL Multiphysics

The governing equation (1) developed for the propulsion mechanism is analyzed as a 1D time dependent PDE in COMSOL Multiphysics mathematical interface.

3.1. Geometry

The length unit is set as nanometers. A 1 dimensional domain was defined as an interval that is equal to the length of the tail expressed as multiple of the characteristic length [7]. This total length i.e. interval is specified as 54650 nm.

3.2. PDE *(g)*

The governing equation (1) is mapped to the general form of the PDE modeling by dividing it into two second-order PDE.

$$EI(x)\frac{\partial^2 p}{\partial x^2} = -\frac{4\pi\mu}{2-\log(\mathrm{Re})}\frac{\partial y}{\partial t} \quad (6)$$

$$\frac{\partial^2 y}{\partial x^2} = p \quad (7)$$

The two dependent variables (p,y) are analyzed using a time dependent study. The boundary conditions are inserted as two Dirichlet boundary conditions (eqn. 2 and 4) and two Flux / source terms (eqn. 3 and 5). The approach is illustrated in the following flow chart (Fig.1).

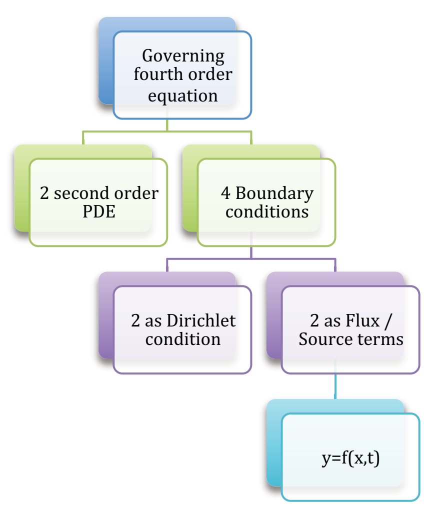

Figure 1. Solving Algorithm

3.3. Meshing

The Meshing is kept to enhance general physics iterations carried over the interval selected in 1D. The maximum mesh element size is also kept in terms of the characteristic length such that the domain is discretized in 100 elements.

3.4. Solver settings

The solver solves for the time dependent problem and gives the solution of transverse displacement at each point on the tail at defined intervals of time. The total cycle time is calculated with respect to the forcing function frequency i.e. 100 rad/s. This comes out to be 0.06283s. The time steps for study are also set such that we get the results in the 8 equal time interval of the cycle time as taken in the literature [7]. Hence the step is set to 0.007854s. The same is set in the solver configuration for the study.

3.5. Parameters

The values of the parameters used are listed in the table below

Table 1. List of Parameters used

Parameters	Expression/Value	Description
Re	0.0001	Reynolds's Number
μ	0.001 Ns/m^2	Viscosity
C	$\frac{-4\pi\mu}{2-\log(\mathrm{Re})}$	Drag Coefficient
ω	100 rad/s	Forcing frequency
G	4E-9	Slope amplitude
A	1E-22 Nm^2	E*I
l_0	$\left(\frac{-A}{C\omega}\right)^{0.25}$	Characteristic length
L	10*l_0	Total length

4. Results

The PDE in (eqn.1) was solved for planar wave configuration of a constant diameter flagellum. The plots of the shape form obtained were in accordance with those published in literature [7] and also corroborates to the damping distance of around 2.6 times the scale length in the waveform. The maximum amplitude of the envelope formed dampens by 30% at this distance.

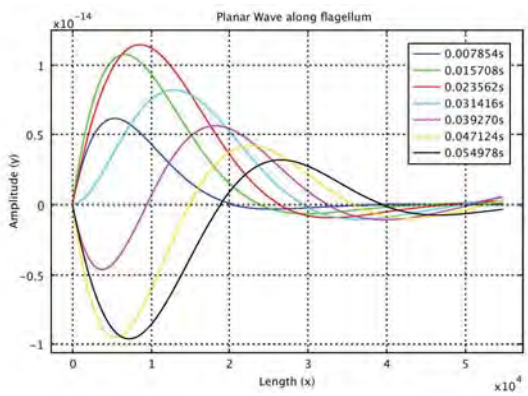

Figure 2. Flagella Shape and Amplitude superimposed for various time steps

Fig.2 represents the variation of wave along the flagellum for various time steps while Fig.3 represents the principal mode of vibration for the planar wave.

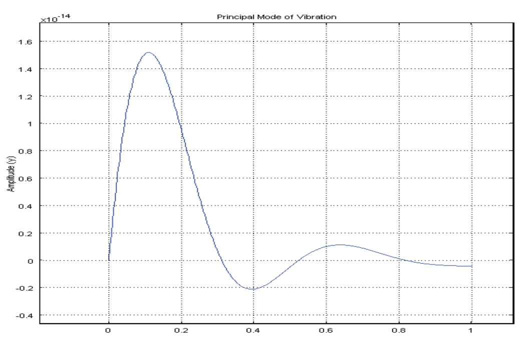

Figure 3. Steady state configuration

5. Conclusions and Future Work

As indicated in Fig.2, the value of damping distance and the wavelength of wave dovetail comply with those proposed in analytic solutions in literature [7]. This study can be further extended for the analysis of varying cross sectional flagella executing planar wave.

6. References

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7. Acknowledgements

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