NUMERICAL SIMULATION OF TWO-DIMENSIONAL MICROORGANISM LOCOMOTION USING THE IMMERSED BOUNDARY METHOD

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가상경계법을 적용한 2차원 미생물 이동에 관한 수치연구

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Study on swimming of microorganisms like, sperm motility, cilia beating, bacterial flagellar propulsion has found immense significance in the field of biological fluiddynamics. Because of the complexity involved, it is challenging for the researchers to model such problems. Immersed boundary method has proved its efficacy in the field of biological fluiddynamics, The present work aims at performing a numerical study on the microorganism locomotion using the immersed boundary method proposed by Peskin[1]. A two-dimensional model of the microorganism is modeled as thin elastic filament described as a sine wave. The neutrally buoyant organism undergoing deformations is immersed in a viscous and incompressible fluid. The fluid quantities are described using Eulerian coordinates and the immersed body is represented by Lagrangian coordinates. The Eulerian and Lagrangian variables are connected by the Dirac delta function. The Navier-Stokes equations governing the fluid flow are solved using the fractional step method on a staggered Cartesian grid system. The developed numerical code in FORTRAN will be validated by comparing the numerical results with the available results.

Key Words : Biofluiddynamics, Microorganism propulsion, Immersed boundary method, Navier-Stokes equation

1. INTRODUCTION

Most of the microorganisms swims in fluid by passing waves of lateral displacement down the body. Phenomenon like motion of a sperm, beating of cilia, bacterial flagellar propulsion, are observed at low Reynolds number whereas aquatic organisms like fish, eel, cetacean etc propels themselves in fluid where the Reynolds number is very high. At high Reynolds number flow, the inertial forces are dominant. But at low Reynolds number, the viscous forces are more significant. The typical Reynolds number for fish and swimming eel are about 10,000 whereas in the case of sperm and bacterial flagellar motion it is about 0.001. Since the swimming of microorganisms are due to the travelling of wave down the body, the relevant parameters related to swimming depends on the amplitude, wavelength and frequency of the travelling wave in addition to Reynolds number of the flow.

This paper presents a computational model which mimics that of a microorganism and we are aimed at studying its propulsion in a viscous and incompressible fluid[2]. The organism is assumed to be massless and elastic. The organism which undergoes deformations within the fluid exerts forces on the fluid and affects the motion of the fluid. This is a typical fluid-structure interaction problem. Hence to simulate such a challenging problem we employed the immersed boundary method proposed by Peskin[1]. Immersed boundary method has proved its ability to handle the simulation of complex flow problems in computational fluid dynamics. Peskin[3] developed the immersed boundary method for the simulation of heart valves. The entire simulation was carried out on a Cartesian grid which did not conform to the geometry of the heart and the effect of immersed boundary on the

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flow was employed through a momentum forcing procedure. Various modifications are made to this method by different researchers emerging it as an efficient numerical tool in handling complex flow simulations in the field of computational fluid dynamics. The main advantage of immersed boundary method is the easiness in grid generation since it employs regular cartesian grid. When compared with the unstructured grid method used for the complex flow problems, the immersed boundary method is proved to be superior in the case of memory and CPU savings.

The immersed boundary method utilizes momentum forcing and a Cartesian grid Navier-Stokes solver. Based on how the momentum forcing is employed in the Navier-Stokes equation, immersed boundary method has been classified into two-continuous forcing approach and discrete forcing approach[4].The discrete version of immersed boundary method employs interpolation techniques to obtain the desired no-slip conditions at the boundary and the momentum forcing is obtained directly from the discretized Navier-Stokes equations[5]. The continuos forcing approach of immersed boundary method utilizes Eulerian vairables for the fluid region and Lagrangian variables for the solid region. The interaction between these two variables are linked by the Dirac delta function. The continuous forcing approach is used for the simulation of fluid-flexible body interaction. For the simulation of elastic bodies interacting with the fluid, the Lagrangian force is the elastic force which can be obtained by applying Hooke's law. But when dealing with rigid bodies, the law is not well posed. Hence in such cases, methods like virtual boundary method proposed by Goldstein et al.[6] is employed. This method is based on the feedback forcing scheme which can enforce the no-slip boundary conditions on the rigid boundary immersed in the fluid. The basic difference between virtual boundary method and that of Lai and Peskin[7] is that, the boundary points are exactly prescribed in the former method, but allowed to move slightly from their equilibrium positions in the latter. Recently, Shin et al.[8] proposed a new version of immersed boundary method which combines the feed back forcing scheme of virtual boundary method along with Peskin's regularized delta function. Huang et al.[9] proposed an immersed boundary formulation simulating flexible filaments in uniform flow. In their simulation, the Eulerian fluid motion and the Lagrangian filament motion were solved independently and their interaction force was explicitly calculated using a feedback law.

The present work is based on the continuous forcing approach of immersed boundary method. We employed the immersed boundary method proposed by Fauci L J and C S Peskin[2]. The computational model presented here is solved in a two-dimensional fluid domain in which the organism undergoing time-dependent undulations is immersed. The organism is modeled as a single filament. Eventhough the flow is viscous dominant we solved the full Navier-Stokes equation considering the inertial effects also. The present work is a preliminary work towards the simulation of bacterial flagellar propulsion and bacterial flagellar bundling.

2. NUMERICAL METHOD

The Navier-Stokes equation for the incompressible viscous fluid flow is given by,

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}.\nabla\mathbf{u}\right) = -\nabla p + \mu\nabla^2\mathbf{u} + \mathbf{f} \tag{1}$$

and the continuity equation is given by,

$$\nabla.\mathbf{u} = 0 \tag{2}$$

where ρ is the density of the fluid, μ is the viscosity of the fluid, p is the pressure and $\mathbf{f}$ is the external force per unit volume applied to the fluid. This force is termed as the momentum forcing function in the Navier-Stokes equation. The external force $\mathbf{f}$ is depended on the position of immersed boundary points and the time. Here, the Eulerian force density $\mathbf{f}(\mathbf{x},t)$ is computed from the Lagrangian force density $\mathbf{F}(s,t)$ as follows:

$$\mathbf{f}(\mathbf{x},t) = \int \mathbf{F}(s,t)\delta(\mathbf{x} - \mathbf{X}(s,t))\, ds \tag{3}$$

The immersed boundary method used in the present work employs an elastic energy function $E(X_k,t)$ to compute the Lagrangian force density $F(s,t)$[2]. The elastic energy function is time-dependent which also depends upon the configuration of consecutive triples of points along the boundary. The Lagrangian force acting on the point Xk is computed from the energy function as its negative derivative with respect to X_k.

$$\mathbf{F}(s,t) = -\frac{\partial E}{\partial \mathbf{X_k}} \tag{4}$$

The elastic energy function is determined as below:

$$E\left(\mathbf{X}_{l,t}\right)=S_1\sum_k\left[\left\|\mathbf{X}_{k+1}-\mathbf{X}_k\right\|-\Delta s\right]^2 + S_2\sum_k\left[\hat{z}.\left(\mathbf{X}_{k+1}-\mathbf{X}_k\right)\times\left(\mathbf{X}_k-\mathbf{X}_{k-1}\right)-C_k\left(t\right)\right]^2 \quad (5)$$

where Δs is the resting length and $\hat{z}=(0,0,1)$ is the unit vector. The above equation signifies that for each immersed boundary point , the energy function has two contributions , energy from stretched springs and energy from bending the entity. The first term in the above equation represents the elastic stretching energy according to Hooke's law of springs. The second term represents the bending energy term. The above two energies are used to used to define the elastic properties of the immersed boundary point. The first term helps in determining the size of the entity and prevent the immersed boundary points from separating far enough to allow the flow to cross the boundary. The second term helps in determining the shape of the immersed boundary , especially they are useful to prevent the boundary from becoming too irregularly shaped near any point. S_1 and S_2 are the stiffness constants which depend upon the arc length Δs and determine how strictly the constraints are enforced. The role of stiffness constants can be viewed in two ways [2]:

(1) Physiological parameters:- The organism's muscular structure will tend to generate a predetermined swimming motion but the effect of the fluid can alter this motion; how much alteration depends on the size of S_1 and S_2.

(2) Numerical parameters:- The swimming motion of the creature relative to itself is completely specified in advance. Then S1 and S2 should be taken as large as possible. The term $C_k(t)$ is the driving function which establishes the shape and time dependence of the swimming motion. But the actual displacement and swimming speed are determined from the fluid flow.

The energy function defined above can be employed to enforce many different configurations, but in the present work we assumed the following configuration,

$$y=a\sin\left(ks-\omega t\right) \quad (6)$$

where a is the amplitude of the wave, k is the wave number and ω is the frequency. For the constant amplitude of the wave, the driving function can be derived as follows[2]:

$$C_k\left(t\right)=-k^2a\Delta s^3\sin\left(ks-\omega t\right) \quad (7)$$

The velocity of a material point of the microorganism is determined from the fluid velocity at that point. A four point Dirac delta function is employed here for the effective transfer of Eulerian and Lagrangian variables. Hence the velocity of material point of the organism is obtained as:

$$\mathbf{U}\left(s,t\right)=\int\mathbf{u}\left(\mathbf{x},t\right)\delta\left(\mathbf{x}-\mathbf{X}\left(s,t\right)\right)d\mathbf{x} \quad (8)$$

where $\mathbf{U}(s,t)$ is the velocity of the immersed boundary point and $\mathbf{u}(\mathbf{x},t)$ is the fluid velocity. Here $\delta(\mathrm{x})$ is the Dirac delta function defined as follows:

$$\delta(\mathbf{x})=\frac{1}{h^2}\phi\left(\frac{x_k-x_i}{h}\right)\phi\left(\frac{y_k-y_i}{h}\right) \quad (9)$$

where $\left(x_k,y_k\right)$ and $\left(x_i,y_j\right)$ are Lagrangian and Eulerian grid points. A four point delta function is employed here for the transformation of quantities between Lagrangian and Eulerian grids.

$$\phi\left(r\right)=\begin{cases}\frac{1}{8}\left(3-2|r|+\sqrt{1+4|r|-4r^2}\right), & 0\le|r|<1\\ \frac{1}{8}\left(5-2|r|-\sqrt{1+4|r|-4r^2}\right), & 1\le|r|<2\\ 0, & 2\le|r|.\end{cases} \quad (10)$$

The computed material point velocity is used for moving the immersed boundary point from its current position to the new position.

$$\frac{\partial\mathbf{X}\left(s,t\right)}{\partial t}=\mathbf{U}\left(s,t\right)$$
$$\mathbf{X}^{n+1}=\mathbf{X}^n+\Delta t\,\mathbf{U}\left(s,t\right) \quad (11)$$

In short, the numerical procedure involves, determining the Lagrangian force density defined on boundary points using the elastic energy function, spreading this force density to the Eulerian grid to get the Eulerian force

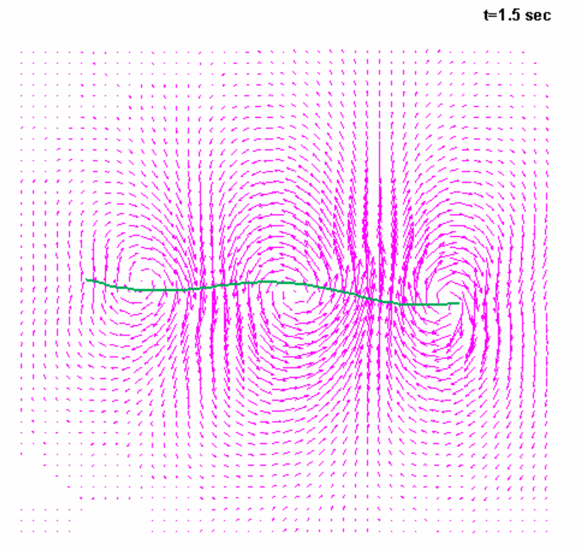

Fig.1 Snapshot of filament and flow field at t=1.5 sec.

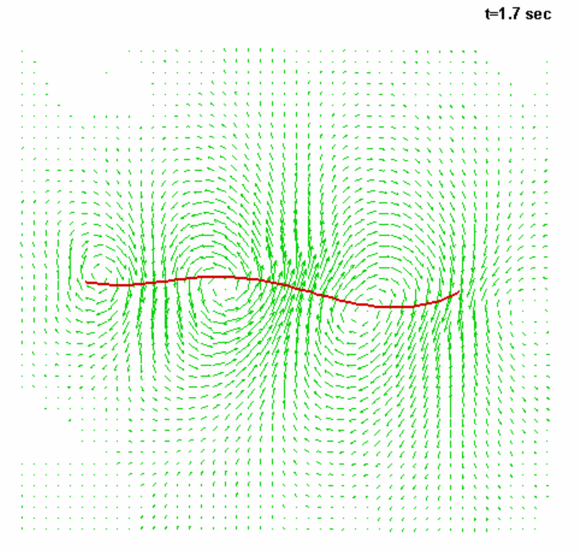

Fig.2 Snapshot of filament and flow field at t=1.7 sec.

density, solving the Navier-Stokes equation to obtain the flow field and then interpolating the fluid velocity field to boundary points and moving the boundary at this local fluid velocity. This completes one time loop.

3. RESULTS AND DISCUSSIONS

In the present work, the swimming of a microorganism of finite length is studied in periodic fluid domain. The flow in X-direction is assumed to be periodic. A square domain of size 0.2cm x 0.2cm is used as the computational domain. The microorganism is modeled as a finite filament in the form of sine wave with the immersed boundary points describing it are initialized to lie along the specified sine wave, with the center line corresponding to the center of the computational domain.

A staggered grid system is adopted here with finite volume discretization for the Navier-Stokes equation. Fractional step procedure in which a pseudo-pressure term is used to satisfy the continuity is employed here for solving the Navier-Stokes equation. We assumed a constant amplitude from the head to tail of the organism. We used a uniform grid system of 64 x 64 for the fluid domain and 128 grid points are used for describing the filament. By employing this, no fluid will be allowed to leak through the immersed boundary points. We set density, $\rho = 1\ gm/cm^3$, viscosity, $\mu = 0.01\ gm/s.cm$, frequency, $\omega = 8\pi s^{-1}$, wave number, $k = 20\pi\ cm^{-1}$ and wavelength, $\lambda = 0.1cm$. The amplitude of the waving motion is considered to be $a = 0.01cm$, which is 10% of the wavelength which seems to be more substantial. The Reynolds number is calculated based on the wavelength which is given by:

$$Re = \frac{\omega}{\nu k^2} \approx 0.6$$

The time period of motion is 0.25 sec. The code is run for eight periods, ie, 2 sec to get a steady periodic state. The stiffness constants S_1 and S_2 are selected in such a way that the filament is almost rigid.

We present the numerical simulation results on the motion of the organism during a particular period of motion. The snapshots of filament and flow field at four different instants during the last period of motion is shown in fig.1-4. The wave propagates over the filament from left to right and the resulting swimming motion is towards the left. It is verified that similar results has been obtained by Fauci L J and C S Peskin[2] in their numerical model which is the basis of this work.

The above numerical simulation results are generated by developing a code in FORTRAN. The present work is under progress. Presently, we are investigating on the proper validation of the developed code by comparing the obtained numerical results with available results. For this, first we will model the filament as an infinite sheet swimming in a periodic fluid domain. Taylor[10], Tuck[11]

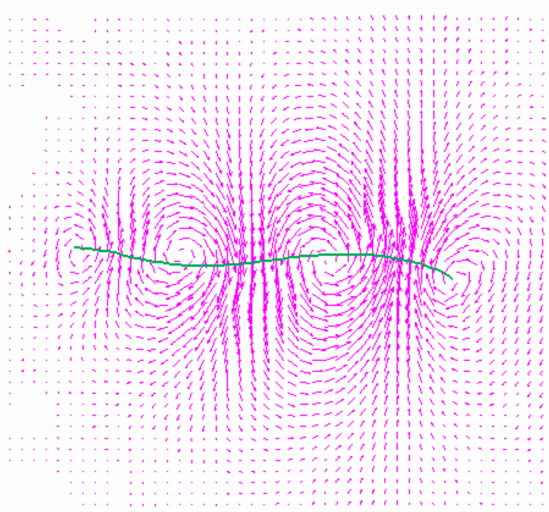

Fig.3 Snapshot of filament and flow field at t=1.8 sec.

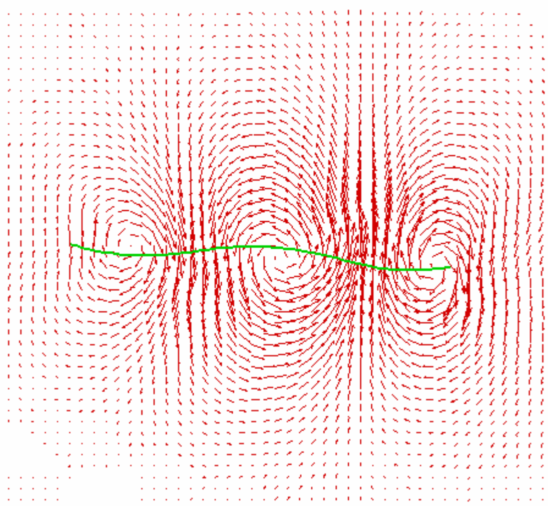

Fig.4 Snapshot of filament and flow field at t=2.0 sec.

and Katz[12] has performed similar studies. Taylor's studies are designed for small amplitude motion, and zero Reynolds number flow, whereas Tuck analyzed the case of small amplitude motion taking inertia into account. Both these studies are limited to small amplitude motions. Katz analyzed the propulsion of an infinite waving sheet parallel to the walls of the channel. Lubrication theory was used to examine the case where the width of the channel was much smaller than the wavelength of the sheet. We are presently performing the above studies based on the present numerical model which will be a good validation of our developed code. The validation results will be presented in the presentation. Also we are focussing on a detailed studies on the swimming phenomenon of the organism with respect to various wave parameters and Reynolds numbers. The results of these studies will be included in the presentation.

4. CONCLUSIONS

The propulsion of a microorganism which is modeled as an elastic massless filament, in an incompressible viscous fluid is studied using the immersed boundary method. A time dependent elastic energy function is used to obtain the necessary forces on the immersed boundary points. A Dirac delta function is used to spread these forces into the fluid region to get the force exerted by the organism on the fluid. The Navier-Stokes equation are solved on a staggered Cartesian grid with finite volume discretization and fractional step method to get the flow velocity field. The obtained fluid velocity is then used to move the organism from its current position to new position. As a result, the wave travels from left to right over the filament during the time and the organism swims towards right. With regard to this, our results matches with the real physical situation of microorganism swimming at low Reynolds number flow. The present study is under progress. The validation of the developed code in FORTRAN by comparing the simulation results for an infinite sheet swimming in the fluid with that of available results and the simulation results based on the various wave parameters and Reynolds number are under investigation. The results of the above studies will be presented in presentation.

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