A Computational Model of the Fluid Dynamics of Undulatory and Flagellar Swimming

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SYNOPSIS. We present a mathematical model and numerical method designed to study the fluid dynamics of swimming organisms. The full Navier-Stokes equations are solved in a domain of fluid within which an organism undergoing time-dependent motions is immersed. Of interest are both the dynamics of a single organism and the relationship of its morphology to its motility properties, as well as the collective hydrodynamic interactions of groups of swimmers with each other and their environment. Biological applications include spermatozoa motility in the reproductive tract, swimming of non-smooth filaments, and collective swimming of algal cells.

INTRODUCTION

The fluid dynamics of aquatic animal locomotion has been studied by zoologists, biologists, engineers and mathematicians. Of interest are both the dynamics of a single organism and the relationship of its morphology to its motility properties, as well as the collective hydrodynamic interactions of groups of swimmers with each other and their environment. The coupled mechanical system consisting of an incompressible fluid and a force-generating organism is, in general, difficult to analyze (Childress, 1981; Lighthill, 1975). The aim of this paper is to show that computational methods may be used to analyze previously intractable problems. Our goal is to make use of modern methods in computational fluid dynamics to create a controlled environment (the computer) where the measurement and visualization of locomotive effects can be made. These effects may include the coupling of organism motility with the advection, diffusion and reaction of a chemical species within the fluid, as well as the hydrodynamic interactions of swimming organisms with each other and surrounding geometries.

Whereas analytical methods work best at the extremes of Reynolds number, our computational method works well at moderate Reynolds numbers. Furthermore, many restrictive idealizations of the geometry of a swimming creature which must be made in asymptotic methods are avoided. The computational creatures need not be infinitely long, nor swim with a constant amplitude from head to tail. In short, the computational approach makes it feasible to study models that are realistic enough to do justice to nature's complexity of design.

We have developed a mathematical model and numerical method designed to study the coupled mechanical system comprised of the fluid and the immersed organism. The full incompressible Navier-Stokes equations are solved in a two-dimensional domain of fluid within which neutrally-buoyant organisms undergoing time-dependent movements are immersed. Fluid quantities are represented on a grid (Eulerian description), and the swimming organisms are modeled by a discrete collection of moving points (Lagrangian description). The salient feature of this technique is that the suspended organism is replaced by suitable contributions to a force density term in the fluid dynamics equations. A single set of fluid equations holds in the entire domain.
and there are no internal boundary conditions. Consequently, the fluid dynamics equations may be solved efficiently using finite-difference methods on a uniform computational grid (Fauci and Fogelson, 1993).

In Section 2, we discuss the mathematical model and numerical method. In Section 3, we present results applicable to two systems: (1) swimming of non-smooth filaments and (2) swimming of algal cells.

**Mathematical Model**

In Fauci and Peskin (1988) and Fauci (1990), we developed a computational model of the swimming of a neutrally-buoyant organism undergoing deformations within a region filled with fluid. This model was adapted from an innovative computational approach, the *immersed boundary method*, which was introduced by Peskin (1977), to model blood flow in the heart. This method has been advanced to study other biofluiddynamic problems including platelet aggregation (Fogelson, 1984), three-dimensional blood flow in the heart (Peskin and McQueen, 1989a, b), dynamics of the inner ear (Beyer, 1992), peristaltic pumping of solid particles (Fauci, 1992), and bacterial chemotaxis in micro pores (Dillon et al., 1995).

The Navier-Stokes equations of motion for a viscous, incompressible fluid in which a neutrally-buoyant, elastic organism is immersed are:

\[
\begin{align*}
\rho \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla p + \mu \Delta \mathbf{u} + \mathbf{F}(x, t) \\
\nabla \cdot \mathbf{u} &= 0 \\
\mathbf{F}(x, t) &= \int f(s, t) \delta(x - X(s, t)) \, ds
\end{align*}
\]

with boundary condition

\[
\frac{\partial X(s, t)}{\partial t} = u(X(s, t), t)
\]

Here \( p \) is the fluid density, \( p \) is pressure, and \( \mu \) is the fluid viscosity. The state of the fluid at time \( t \) is given by its velocity field \( u(x, t) \) and the state of the immersed boundary (organism) is given by the configuration of the material points \( X(s, t) \). Here \( s \) is an arclength parameter. Equation (1) is Newton’s second law: mass times acceleration equals force. The forces which appear are those due to pressure, viscosity and the external force \( \mathbf{F}(x, t) \). This external force represents the force of the organism on the fluid. As expressed in Equation (3) by the Dirac delta function \( \delta \), this external force is a delta function layer of force supported only by the region of fluid which coincides with material points of the organism; away from these points the external force is zero. Equation (2) says the fluid is incompressible, and equation (4) is the *no-slip* boundary condition, which says that the velocity of a material point of the organism is equal to the velocity of the fluid at that point.

The external force establishes the presence of the immersed boundary in the fluid. It is through this term that the forces generated by the organism are felt. These forces arise from internal organism mechanics, *i.e.*, active and passive tissue properties, muscle mechanics (Jordan, 1994), or in the case of cilia and flagella, the action of the molecular motor dynein upon the microtubules within an axoneme.

In this simplified model, the boundary forces contributing to \( f(s, t) \) at a material point of the elastic organism \( X(s, t) \) are of two types:

1. A spring-like force which asks that the ‘links’ between successive material points resist compression or expansion from a given arclength.
2. A bending-resistant or hinge-like force which asks that the curvature at a material point be a given function which changes with position and time.

Associated with both the spring and hinge forces are stiffness constants. These stiffness constants can be chosen to reflect physical properties of the organism, *i.e.*, Young’s modulus of elasticity of the tissue. Although we specify the equilibrium, or target configuration of the organism, the organism reacts to drag forces acting on it through the viscous fluid. The higher the stiffness constants, the less impact the drag forces have. In addition, only the equilib-
rium configuration of the organism relative to itself is specified—the actual displacement relative to the fluid domain is not preset, but is determined by the coupled equations of motion.

For numerical implementation of this model, the fluid domain is covered with a rectangular grid on which we define fluid quantities such as velocity and pressure. The immersed boundary is represented by a discrete collection of moving points. These points do not coincide with grid points.

The boundary force is spread to the grid by means of a discretized delta function (approximation of Equation [3]) to calculate the external force field. The fluid quantities are updated by calling a subroutine which integrates the Navier-Stokes equations for one time step on a regular grid. Once the Navier-Stokes equations are solved, the local fluid velocity is interpolated to the immersed boundary using the discretized delta functions. The boundary is then moved at this local fluid velocity. This completes one time step. (For details, see Fauci and Fogelson [1993] and Peskin [1977].) Our immersed boundary is not our computational boundary in the Navier-Stokes solver, but a singular force field which alters the equation just via the right-hand-side. There is no need for complicated discretization of derivatives at grid points near the immersed boundary or boundary conditions which change with time. We are able to model complicated motions with a Navier-Stokes solver designed for a regular mesh with simple boundary conditions.

There is no inherent restriction upon the Reynolds number using this approach. In the present implementation, the Navier Stokes equations are solved on a finite-difference grid. Of course, in order to resolve the small boundary layers related to very high Reynolds number flow, a prohibitively small mesh size would be needed. However, simulations of moderate Reynolds numbers of a few hundred are not problematic. In addition, since the immersed boundary approach is modular, one can use a fluid solver designed for high Reynolds number flow. In particular, grid-free methods have been used in conjunction with immersed, elastic structures (Cortez, 1996).

Although the above discussion describes the modeling of a single immersed organism, additional immersed organisms may be included in the same fluid domain, each contributing to the external force. Figure 1 shows a snapshot of several spermatozoa in a channel. The fluid velocity field at grid points is depicted, as well as the positions of the immersed organisms. This biological system is discussed further in Fauci and McDonald (1995).

**Simulations**

Non-smooth filaments

The principal means of aquatic (eucaryotic) animal locomotion is to pass waves of lateral displacement down the body. This is observed in creatures of all sizes; eels, fish, worms and flagellated microorganisms such as spermatozoa. The propulsive wave passes from front to back, thereby propelling the organism in the opposite direction. There are, however, cases of undulatory motion whereby the organism swims in the same direction as that of the wave. The microorganism *Ochromonas* propels itself by means of a long flagellum with waves propagating in the same direction as the direction of swimming. This hispid flagellum is not smooth, but has many hair-like projections called mastigonemes or thinner filaments (Alexander, 1982). These mastigonemes lie in the plane of beating of the undulating flagellum, and appear to be quite rigid and oriented normal to the flagellum (Brennen, 1976; Taylor, 1952). The rigidity of the mastigonemes is essential to the reversed swimming direction. Other flagella (Euglena) with flexible mastigonemes swim in the opposite direction as the propulsive wave (Brennen, 1976).

On a larger length scale, polychaete worms also swim in the same direction as that of the wave. These annelids have parapodia, hair-like appendages attached to each body segment. Unlike the *Ochromonas*’ mastigonemes, these parapodia are not passive, but, also exhibit wave-like rowing motions (Clark and Tritton, 1970; Gray, 1939). Here, the Reynolds number is not
FIG. 1. Six spermatozoa swimming in a channel. Since a swimming organism is represented by a suitable contribution to the external force field in the fluid dynamics equations, more than one organism is easily included in the same domain. Their interactions are mediated through the fluid. The arrows depict the direction and magnitude of the fluid velocity field. Note that in this simulation, the channel walls are also represented as immersed boundaries, and there is fluid present outside as well as inside the channel. The velocity field is zero outside the channel.

near zero, as is the case for microbes, but can range from order one to order 20,000 depending upon the size of the organism.

We have constructed a computational creature consisting of a central filament, from which sixteen "hairs" emanate. A sine wave propagates from left to right (Fig. 2). This organism swims at a Reynolds number of approximately 4, based upon wavelength and wavespeed. The amplitude of its oscillation is small; about 6 percent of its wavelength. Figure 3 shows a snapshot of the flow field and the immersed creature.

By varying the stiffness constants associating with bending rigidity, the "hairs" can be modeled as rigid or flexible. We have performed calculations for three cases. In the simulations exhibited in Figures 2 and 3, the bending rigidity of the append-
FIG. 2. Position of filament during a single period. These are positions of the filament during equally-spaced time intervals. The appendages contribute strong bending resistant forces to the fluid. The dot indicates the position of the crest of the wave, with the organism providing the frame of reference. Note the wave passing from left to right.

ages was large. In the second case, there was no bending rigidity applied by the flexible appendages, but their presence did contribute elastic spring forces to the fluid. Finally, we performed a calculation using the same parameters as in the first two cases, but did not include any appendages on the immersed creature. The results of the swimming progression in each case is shown in Figure 4. Note that the smooth filament makes progress towards the left. The filament with rigid appendages progresses towards the right, as expected. The filament with flexible appendages progresses, rather slowly, towards the left. Some contribution of bending stiffness or rigidity was necessary for reversal of swimming direction.

One can use this computational tool to determine the effects of the distribution, length, and stiffness properties of the appendages on the overall swimming direction, speed and energy requirements. In addition, the appendages can be made to actively row, so as to model the parapodia of polychaetes.

Algal cells

Biflagellated algal cells, *Chlamydomonas* in particular, have been studied in the context of phototaxis, the orientation of movement with respect to light (Nultsch, 1983), and geotaxis, the orientation of movement with respect to gravity (Kessler, 1985, 1986, 1989). The mechanics and hydrodynamics of locomotion are central to the understanding of these phenomena.

These algal cells are unicellular organisms consisting of a cell body and two an-
terior flagella. They swim using power/recovery strokes of two anterior flagella (much like the beating of cilia). During the power stroke, the two flagella are held fairly straight and beat backwards. During the recovery stroke, a bending wave propagates from the base of the flagella to the tip (Ruffer and Nultsch, 1985).

We have successfully simulated this mode of swimming in two dimensions (Fauci, 1993). The cell body is made up of a ring of points, and is mechanically coupled to two flagella, which row and periodically change their curvature. Figure 5 shows results of calculations where two algal cells are immersed in the same fluid domain. The cells are made to beat in synchrony.

In our simulations of algal cells thus far, the organism is taken to be neutrally-buoyant. In reality, however, the density of these microorganisms is about five percent more than that of water. They tend to swim against gravity (negative geotaxis) because their cell bodies are 'bottom heavy' due to the position of the chloroplast. Moreover,
SWIMMING FILAMENTS
WAVE TRAVELS LEFT TO RIGHT

Fig. 4. Swimming progression of different filaments. The wave passes from left to right with a period of 0.25 seconds. Note that the smooth filament and the filament with flexible appendages swim in the opposite direction as the wave, but the filament with rigid appendages swims in the same direction as the wave. (In each case, at time t = 0, the amplitude of the filament was zero, but within a few time steps the amplitude reached its constant level. This was done to simplify the numerical initialization of appendages.)

this geotaxis is vorticity-sensitive in that a local rotation of the flow tends to incline the swimming axis by an amount which depends upon the distance between the center of volume and the center of mass (Kessler, 1985, 1986, 1989). Kessler has demonstrated focusing of Chlamydomonas towards the axis of down-flowing fluid in a pipe, and towards the periphery of the pipe when the fluid is flowing upwards.

Our hope is to include the effects of differing densities along the cell body by distributing applied gravitational forces along the immersed boundary. Also of interest is the phenomena of bioconvection—the formation of patterns due to the suspension of negatively geotactic organisms (Kessler, 1985, 1986, 1989; Pedley and Kessler, 1992). While we cannot hope to represent thousands of discrete microorganisms computationally at the above level of detail, we can realistically represent a small group (2–100) of organisms. There is still much to be learned about the details of the fluid dynamical interaction of neighboring algae. This can then be coupled with a larger-scale model which represents the algae as a continuous distribution.

CONCLUSION

In this paper, we have outlined a mathematical model and numerical method designed to study the coupled mechanical system of an incompressible fluid and force-generating organisms. This experimental tool can be used by biologists to explore the effect of different parameters (fluid viscosity, undulatory wave speed and amplitude, beat frequencies of flagella, etc.) upon overall swimming speed and energy requirements. The calculations can be computer-intensive, but may be performed on desk-top workstations.
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Fig. 5. Two algal cells in same domain. Velocity fields and positions of organisms during three phases in a single beat period. The final frame shows superimposed organism positions during this period.
COMPUTATIONAL MODEL OF SWIMMING


