Singularity methods and slender body theory

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How many of us have been in the kitchen, chopping an onion, when suddenly we're chopping our finger? When this happens, the body rapidly responds. Cells mobilize to fill the gap, and eventually a scab forms, which gives way to new skin. While this process is simple to observe, it is quite complicated beneath the surface. Cells have to move rapidly into the open wound, which requires them to transport their large nuclei. To do this, cells deform the thousands of long slender filaments that make up their cytoskeleton.

This report is about some simple mathematical ways to understand the movement of cells. In particular, we discuss singularity methods for fluid flow problems. We begin by introducing the PDEs that govern fluid flows inside of cells. Then we discuss the fundamental singularities that can form solutions to the PDEs. We finish with two applications: fluid flow due to a translating sphere (a model of the nucleus) and a translating slender fiber (the type of fiber that makes up the cell cytoskeleton).

1 Fluid equations

The cell is made up of structures called organelles immersed in a fluid with properties similar to those of water. The flow of the fluid exterior to the structures can be described by the three-dimensional incompressible Navier-Stokes equations

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t}+\boldsymbol{u}\cdot\nabla\boldsymbol{u}\right)=\mu\Delta\boldsymbol{u}-\nabla p+\boldsymbol{f}, \tag{1}$$

$$\nabla\cdot\boldsymbol{u}=0. \tag{2}$$

Here ρ is the density of the fluid, the vector $\boldsymbol{u}$ is the fluid velocity, p is the fluid pressure, μ is the fluid viscosity (how resistant the fluid is to motion), and the vector $\boldsymbol{f}$ is any external force density applied to the fluid, for example gravity. The symbol Δ denotes the vector Laplacian. Equation (1) is a statement of momentum conservation and can be derived by setting the rate of change of momentum in a moving volume of fluid to zero. Likewise, Eq. (2), which is known as the incompressibility condition, is a statement of mass conservation in a constant density fluid. Mathematically, the pressure p is a Lagrange multiplier that enforces the incompressibility and can be eliminated via a Schur complement approach. For this reason, we focus in this report on the solutions for the velocity $\boldsymbol{u}$.

The left-hand side of the momentum balance (1) is the acceleration of a fluid parcel and is negligible when the problem length scales are small and the viscosity μ is large. Imagine trying to move micrometer distances through thick oil sludge. The acceleration is so small in this case that it can be safely neglected, and the system is in a steady state dictated uniquely by the forcing $\boldsymbol{f}$. The momentum balance equation reduces to the right-hand side of momentum balance (1),

$$0=\mu\Delta\boldsymbol{u}-\nabla p+\boldsymbol{f}. \tag{3}$$

The mass conservation equation, (2), is unchanged. Thus the system of PDEs that describe fluid flow inside the cell is given by Eqs. (2) and (3). These are called the *Stokes equations.*

2 Fundamental solutions

Having stated the relevant fluid equations in cell biology, we next seek to solve them in the presence of the cell organelles, such as the nucleus and cytoskeleton. Suppose for example that we model the nucleus as a sphere moving with a constant velocity. Then we need to solve fluid equations (2) and (3) for $\boldsymbol{u}$, subject to the boundary condition that the fluid velocity on the surface of the sphere is equal to the rigid body velocity of the sphere (this is called the *no-slip* boundary condition). This problem has a simple solution that can be determined by the so-called *method of singularities.* In this section, we define and develop this method so we can use it in Section 3 to solve fluid flow problems.

Since the momentum balance (3) is a linear equation in $\boldsymbol{u}$, solutions can be constructed by superposition of fundamental solutions known as singularities. To derive one of these singularities, suppose that we solve the Stokes equations (2) and (3) with $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{f}_0 \delta(\boldsymbol{x} - \boldsymbol{x}_0)$ being a point force with strength $\boldsymbol{f}_0$ at $\boldsymbol{x}_0$. Then the solution for the velocity is

$$\boldsymbol{u}(\boldsymbol{x}) = \frac{1}{8\pi\mu} \left(\frac{\boldsymbol{I}}{\|\boldsymbol{r}\|} + \frac{\boldsymbol{r}\boldsymbol{r}^T}{\|\boldsymbol{r}\|^3} \right) \boldsymbol{f}_0 := \boldsymbol{S}(\boldsymbol{x}, \boldsymbol{x}_0) \boldsymbol{f}_0, \tag{4}$$

where $\boldsymbol{I}$ is the identity matrix, $\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{x}_0$, and we have defined a matrix $\boldsymbol{S}(\boldsymbol{x}, \boldsymbol{x}_0)$ which is called a *Stokeslet* centered at $\boldsymbol{x}_0$. The velocity due to the Stokeslet satisfies the homogeneous Stokes equations, (2) and (3), with $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{0}$ for $\boldsymbol{x} \neq \boldsymbol{x}_0$. At $\boldsymbol{x} = \boldsymbol{x}_0$, the velocity is undefined (singular).

In this sense, if we consider the fluid domain except at $\boldsymbol{x} = \boldsymbol{x}_0$, we can construct more solutions to the Stokes equations by taking derivatives of the Stokeslet. For example, if we take the Laplacian of the Stokeslet, we obtain a solution that is called the doublet,

$$\boldsymbol{D}(\boldsymbol{x}, \boldsymbol{x}_0) = \Delta_{\boldsymbol{x}} \boldsymbol{S}(\boldsymbol{x}, \boldsymbol{x}_0) = \frac{1}{8\pi\mu} \left(\frac{\boldsymbol{I}}{\|\boldsymbol{r}\|^3} - 3\frac{\boldsymbol{r}\boldsymbol{r}^T}{\|\boldsymbol{r}\|^5} \right). \tag{5}$$

Like the Stokeslet, the doublet satisfies the homogeneous Stokes equations for $\boldsymbol{x} \neq \boldsymbol{x}_0$ and is undefined at $\boldsymbol{x} = \boldsymbol{x}_0$. Because the Stokeslet and doublet are singular at $\boldsymbol{x} = \boldsymbol{x}_0$, they are two of the so-called fundamental *singularities* for Stokes flow.

3 Using singularities to solve BVPs

3.1 Flow outside a sphere

Let us return now to our motivating model of the nucleus as a translating sphere in Stokes flow. We denote the spherical nucleus by S and its surface by ∂S. Suppose that S is of radius a, and, at a fixed moment in time, is centered at $\boldsymbol{x}_0$ and moving with velocity $\boldsymbol{U}$. The equations to solve are the homogeneous Stokes equations outside the sphere,

$$\mu \Delta \boldsymbol{u} - \nabla p = 0 \quad \text{on } \mathbb{R}^3 \setminus S, \tag{6}$$

$$\nabla \cdot \boldsymbol{u} = 0 \quad \text{on } \mathbb{R}^3 \setminus S. \tag{7}$$

On the surface of the sphere, we assume a no-slip boundary condition, so that the fluid has to move at the same velocity as the sphere

$$\boldsymbol{u}|_{\partial S} = \boldsymbol{U}. \tag{8}$$

While these equations appear complex, they actually admit a simple singularity solution. In particular,

$$\boldsymbol{u}(\boldsymbol{x}) = 6\pi\mu a \left(\boldsymbol{S}(\boldsymbol{x}, \boldsymbol{x}_0) + \frac{a^2}{3} \boldsymbol{D}(\boldsymbol{x}, \boldsymbol{x}_0) \right) \boldsymbol{U} \tag{9}$$

is the solution to the boundary value problem (6)−(8) [2, Eq. (43)]. The method we use to construct this solution is universal to singularity methods: we begin with the simplest singularity, in this case the Stokeslet centered at $\boldsymbol{x}_0$. We evaluate the velocity $\boldsymbol{S}(\boldsymbol{x}, \boldsymbol{x}_0)\boldsymbol{U}$ for $\boldsymbol{x}$ on the sphere surface ∂S and determine how much this velocity differs from the sphere velocity $\boldsymbol{U}$. Then, we add the correct coefficients (also called *strengths*) in front of the Stokeslet and higher-order doublet singularity so that the boundary condition (8) is satisfied exactly on the sphere surface. Notice that we only need to worry about the boundary condition here; since the Stokelet $\boldsymbol{S}$ and doublet $\boldsymbol{D}$ in the solution (9) are centered at the sphere center, they are non-singular outside the sphere and therefore satisfy the momentum balance (6) and incompressibility condition (7) by construction.

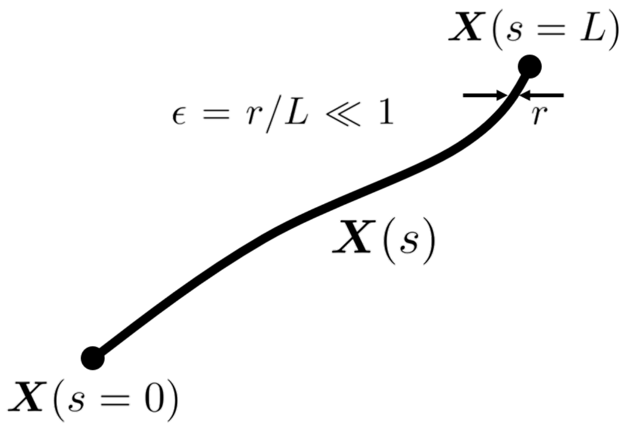

Figure 1: Parameterization and geometry of the fiber F.

3.2 Flow outside a fiber: slender body theory

While the solution for a sphere is both a simple and useful example of singularity methods, many of the shapes we encounter in and around the cell are far from spherical. For example, the cytoskeleton of the cell is made of long, thin, inextensible filaments that control the cell's shape and movement mechanisms [1]. Biological microorganisms also use long, thin flagella to propel their motion inside a fluid [6]. In the 1970s, the desire to study these geometries led to the development of new singularity methods for slender filaments known collectively as *slender body theory.*

The principle of slender body theory is similar to that of the singularity solution for a sphere. Define a fiber F with length L and constant radius r. The aspect ratio of the fiber is $\epsilon = r/L$, and we are interested in the case $\epsilon \ll 1$. As shown in Fig. 1, the centerline of the fiber is parameterized by $\boldsymbol{X}(s)$ with $s \in [0, L]$. We suppose that the fiber is translating with position-dependent velocity $\boldsymbol{U}(s)$, and that this velocity is constant on each cross section. To obtain the fluid flow due to the fiber, we need to solve the system

$$\mu \Delta \boldsymbol{u} - \nabla p = 0 \quad \text{on } \mathbb{R}^3 \setminus F, \tag{10}$$

$$\nabla \cdot \boldsymbol{u} = 0 \quad \text{on } \mathbb{R}^3 \setminus F, \tag{11}$$

$$\boldsymbol{u}|_{\partial F} = \boldsymbol{U}(s). \tag{12}$$

This system is similar to that for a sphere, with the exception of the boundary condition (12), which states that the velocity of the fluid must be equal to the translation velocity of the fiber along its surface. This system is much more challenging than the spherical case, since the translation velocity $\boldsymbol{U}$ changes along the filament.

One way to make the boundary value problem (10)−(12) tractable is to relax the equality in the boundary condition (12). Instead of having the equality hold exactly, suppose we have it hold up to a correction of size roughly ϵ, which is much less than one. This problem also admits a singularity solution, but of a different kind. To obtain it, we place a line of Stokeslets and doublets along the fiber centerline. We choose the doublet strength relative to the Stokeslet strength so that the fluid velocity is constant to $\mathcal{O}(\epsilon)$ on every cross section [3]

$$\boldsymbol{u}(\boldsymbol{x}) = \int_0^L \left(\boldsymbol{S}(\boldsymbol{x}, \boldsymbol{X}(s)) + \frac{r^2}{2} \boldsymbol{D}(\boldsymbol{x}, \boldsymbol{X}(s)) \right) \boldsymbol{f}(s)\, ds. \tag{13}$$

This leaves an unknown Stokeslet strength $\boldsymbol{f}(s)$. In order to obtain it, we evaluate the velocity (13) on the fiber surface asymptotically in ϵ. Since $\boldsymbol{u}(\boldsymbol{x})$ is constant to order ϵ on the fiber surface, it is not important which part of the fiber surface (for constant s) is used to evaluate the velocity. A matched asymptotic procedure gives the velocity on the fiber surface for each s in terms of the Stokeslet strength $\boldsymbol{f}(s)$,

$$\frac{1}{8\pi\mu}\left(\log\left(\frac{4s(L-s)}{r^2}\right)\left(\boldsymbol{I}+\boldsymbol{X}_s(s)\boldsymbol{X}_s(s)^T\right)+\left(\boldsymbol{I}-3\boldsymbol{X}_s(s)\boldsymbol{X}_s(s)^T\right)\right)\boldsymbol{f}(s) \qquad (14)$$
$$+\int_0^L\left(\boldsymbol{S}(\boldsymbol{X}(s),\boldsymbol{X}(s'))\boldsymbol{f}(s')-\frac{\boldsymbol{I}+\boldsymbol{X}_s(s)\boldsymbol{X}_s(s)^T}{8\pi\mu|s-s'|}\boldsymbol{f}(s)\right)ds',$$

where $\boldsymbol{X}_s = \boldsymbol{X}'(s)$ is the fiber tangent vector at s. We now impose the boundary condition (12) to obtain the Stokeslet strength $\boldsymbol{f}(s)$. Specifically, setting expression (14) equal to $\boldsymbol{U}(s)$ for each s gives an integral equation for $\boldsymbol{f}(s)$. The solution of this integral equation can then be used in the velocity equation (13) to obtain the fluid velocity everywhere due to the fiber [3, 5, 4].

There are some caveats, however. First, the leading order term in expression (14), $\log\left(4s(L-s)/r^2\right)$, is singular at $s = 0, L$. This must be treated with some regularization [7], or with more detailed assumptions about the fiber geometry [4]. Second, the integrand in expression (14) is singular at $s = s'$, and so advanced numerical methods must be used to compute it accurately.

4 Conclusion

Singularity methods can greatly simplify the analysis of three-dimensional fluid flows inside the cell. If we model the cell's nucleus by a sphere and its cytoskeleton by a collection of slender fibers, singularity methods give solutions for the fluid velocity inside the cell and consequently its dynamic movement. With singularity methods, we can simulate important biological processes like cell division, wound healing, and cancer growth and gain insights into how the viscous fluid inside the cell impacts each of these processes. For example, if the cell reassembles the cytoskeleton at its rear, do the resulting fluid flows cause the cell to move? When we cut ourselves in the kitchen, what role does the fluid inside the cell play in forming the scab? Answers to these questions are readily attainable with singularity methods.

References

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