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Numerical Computation of Doubly-Periodic Stokes Flow Bounded by a Plane with Applications to Nodal Cilia

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Abstract. A numerical method is presented for the computation of externally forced Stokes flows bounded by the plane $z=0$ and satisfying periodic boundary conditions in the x and y directions. The motivation for this work is the simulation of flows generated by cilia, which are hair-like structures attached to the surface of cells that generate flows through coordinated beating. Large collections of cilia on a surface can be modeled using a doubly-periodic domain. The approach presented here is to derive a regularized version of the fundamental solution of the incompressible Stokes equations in Fourier space for the periodic directions and physical space for the z direction. This analytical expression for $\hat{\mathbf{u}}(k,m;z)$ can then be used to compute the fluid velocity $\mathbf{u}(x,y,z)$ via a two-dimensional inverse fast Fourier transform for any fixed value of z. Repeating the computation for multiple values of z leads to the fluid velocity on a uniform grid in physical space. The zero-flow condition at the plane $z=0$ is enforced through the use of images. The performance of the method is illustrated by numerical examples of particle transport by nodal cilia, which verify optimal particle transport for parameters consistent with previous studies. The results also show that for two cilia in the periodic box, out-of-phase beating produces considerable more particle transport than in-phase beating.

AMS subject classifications: 76D07, 76Z99, 92-08

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1 Introduction

We present an efficient numerical model for the three-dimensional flow generated by carpets of cilia by considering an arrangement that is periodic in two space dimensions.

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Cilia are hair-like structures that attach to the surfaces of cells and move the surrounding fluid through coordinated beating. Cilia perform important functions such as transporting mucus in the lungs and sinuses as well as helping fluid exchange in the ventricles of the brain [6, 30]. Inspired by their role in nature, recently cilia have been integrated into micro-fluidic devices for fluid pumping and mixing [13]. In many applications it is crucial to analyze the fluid flow close to the individual cilium, which requires a detailed model with fine resolution. On the other hand the fluid flow around a cilium is significantly influenced by the motion of surrounding cilia, which requires a larger scale. For instance, cilia can transport fluid more efficiently if instead of beating in perfect synchrony there is a slight phase difference between neighboring cilia (metachronal wave). Numerical models, therefore, have to incorporate the effects of large arrays of cilia while at the same time allowing to resolve individual cilia accurately.

An early approach to model large-scale effects of ciliary carpets is Blake's envelope model, that views the tips of densely packed cilia as a continuum (envelope) [4]. This model was not intended to resolve the region below the cilia tips, which is, for instance, crucial for fluid mixing. Liron and Mochon average the velocity field in one spatial direction [29], which allows for better resolution than the envelope model although the flow field is not fully three dimensional. Some methods model ciliary arrays by computing large numbers of individual cilia. The fluid flow is then analyzed in the middle section of the computational domain in order to avoid edge effects. Smith et al. [35, 36] and Ding et al. [14] represent cilia by a Stokeslet distribution where the point forces exerted by the cilium are found from a prescribed cilium shape. In this approach the forces are the solution of a linear system, the size of which is proportional to the total number of cilia and the number of point forces per cilium. The system can, therefore, be quite large especially for two-dimensional arrays. Gueron et al. assume more flexible beat patterns that change based on multi-cilia interactions and internal mechanisms of cilia and compute one and two-dimensional arrays of cilia [19–21]. They note, however, that some wavelike patterns that require more rows could not be computed due to the prohibitive computational cost [19].

The motivation for focusing on two-dimensional periodicity is to avoid the computational cost associated with computing large numbers of individual cilia. Instead we use only a few cilia, for instance comprising one metachronal wave length, and place them inside a doubly-periodic box. It should be pointed out that besides just saving computational time, periodic boundary conditions can also profoundly change fundamental properties of the system. Lenz and Ryskin, who analyzed analytically and numerically the evolution of the phase difference between neighboring cilia in one-dimensional arrays [28], found that for general beat patterns the metachronal wave is unstable for free boundary conditions but stable for periodic boundary conditions. A number of numerical methods use periodic boundary conditions to model ciliary arrays. Elgeti and Gompper imposed periodic boundary conditions for two-dimensional arrays of cilia using multiparticle collision dynamics, where the fluid is represented by point particles with unit mass [16]. Mitran modeled rows of pulmonary cilia using a flexible grid around each