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Modeling and simulation of active suspensions containing large numbers of interacting micro-swimmers

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ABSTRACT

We present a mathematical model and simulation method to compute the colonial dynamics of micro-swimmers that interact directly and through the fluid they are suspended in. The model uses the stress generated by each self-motile particle for long-range interactions and includes short-range steric effects between particles. The time-step computational cost is $O(N \log N + M)$, with N the total number of mesh points, and M the number of swimmers. This fast method enables us to efficiently simulate many thousands of interacting self-propelling particles in three dimensions and with background flows. We show examples of collective behavior in suspensions of "pusher" and "puller" micro-swimmers.

1. Introduction and motivation

In recent years many experiments and studies have focused on the collective dynamics of self-propelling or types of "active" micro-particles and how they interact with the fluid they live in (see reviews [25,29,32]). The study of a single microorganism's locomotion is an interesting question by itself, as many employ unusual strategies to propel themselves in an environment where inertia is negligible and the viscous effects dominate. The motion of a "suspended" swimming microorganism disturbs the surrounding fluid, and as such it affects the other microorganisms in it, in effect making it possible for the micro-swimmer to interact with the other through it. Capturing the interactions between the organism and the fluid is challenging by itself. In a suspension or many such "active" particles interesting dynamics emerge, such as macroscopic organization and complex flows in which the transport and mixing properties are altered by the micro-swimmers' collective motion. In experiments it is observed that colonies of *Bacillus subtilis* or *Escherichia coli* organize into large-scale structures, and the disturbed fluid flow exhibits vortices and jets with speeds much larger than the swimming speed of any individual bacterium [5,9]. These structures emerge as a result of the interactions between the micro-swimmers, direct or via the surrounding fluid flow, and they depend on the type of swimmer involved as well as the population concentration. The structures are complex and can be influenced by many things, such as internal or external chemical cues, temperature changes, gravity, light, boundaries, etc.

Direct simulations of suspensions of micro-swimmers that capture physically correct individual motions and interactions are desirable in order to study and understand the underlying mechanisms that drive the collective dynamics, but such simulations are difficult because of the very large number of swimmers that have to be individually traced. Numerical simulations that capture particle–particle and particle–fluid interactions at various levels of approximations have been undertaken, e.g. boundary integral methods [31] for two ellipsoidal swimmers [23], simple dumbell models [15,16] or slender-body models for far-field interactions [33], Stokesian dynamics of "squirmers" that propel by a surface slip velocity [19,20,11], immersed boundary method [7,18] or the method of regularized Stokeslets for non-interacting swimmers [1], etc. These simulations can often capture qualitative features observed in experiments, e.g. the large-scale flows and enhanced passive diffusion, and often elucidate details of the interactions between two or more micro-swimmers. The difficulties are however twofold: modeling of the physics and computation. For example, modeling the dynamics of slender self-propelling particles in slow viscous flow using a boundary integral, e.g. [23], yields good resolution and understanding of the flow field close to the body, but local refining is needed when two swimmers get very close, making the method expensive for simulations of many particles. Capturing the direct interaction of the particles in this case is desirable, but it comes at a high computational cost even with modern computational tools. Other methods [33,35] employ far-field interactions only, with the particles feeling the collectively-generated flow,

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but not the neighbors, and as such can overlap and cross with each-other. Typically most direct simulations of suspensions are limited with regard to the number of swimmers, from a few dozen in [11] to a few thousand swimmers even if the local drag approximation (far-field interaction via fluid) is used [35].

It is thus desirable to design a numerical method that captures the physical dynamics a large number of micro-swimmers that interact with each other and with the macroscopic fluid flow, but at a manageable computational cost. To do this we use what is known about the swimming micro-mechanics of a slender motile particle, the far-field fluid flow it generates and how it interacts with nearby swimmers. Each swimmer self-propels, is advected and rotated by the macroscopic flow, but also the disturbance flow it generates due to locomotion. The swimmers in this model interact directly with the neighbors, and also through the fluid flow: hence the interactions are both *steric* and *hydrodynamic*. The locomotion-induced far-field flow, which to the leading order is a force-dipole or stresslet, captures well what is observed in experiments of bacteria like *E. coli* or green-algae *Chlamydomonas reinhardtii* [10]. In low Reynolds number flows the contributions of all the micro-swimmers to the flow can be "added up" to result in a collectively-generated flow field. By stitching together the analytically-obtained leading-order forms in the dynamics of the micro-swimmers, we create a hybrid simulation method that qualitatively captures the suspension dynamics observed in more-involved simulation methods, but with less computational cost, the ability to trace a significantly larger number of swimmers, and the versatility to add to a variety of other types of interactions, particles, boundaries, etc.

In this study we present a mathematical model based on the mechanics of a motile slender particle in a low Reynolds number flow, and also the pair interactions that result from closeness and collisions of two such particles. We describe how to calculate the extra stress generated by many such self-propelling particles and how that can be included in the fluid equations. The numerical method employed uses some of the framework of the immersed boundary method for fluid–structure interactions [30]. We discuss how the model captures the dynamics of one or two interacting self-motile particles, and how this depends on the type of the swimmer propulsion mechanism. The collective behavior of a very large number of micro-swimmers is shown for a variety of swimmer-types at significant swimmer volume fractions or concentrations. We also present one example of many interacting self-propelling particles in a large vortical flow to illustrate the effects of coupling the swimmer dynamics to an external flows much larger in scale and speed than the individual swimmer. In the end, we briefly discuss how the method can be extended to account for other types of interactions between micro-swimmers or other types of active particles.

2. Mathematical model

2.1. Idealized swimmer model

We consider a slender motile non-inertial object that is immersed in a Newtonian Stokes fluid. The simplest and most popular far-field model of slender body theory [3,24,22] is the non-local drag approximation, which is a leading-order dynamics of the swimming dynamics of a Stokesian object. Denoting the object centerline by $\mathbf{Y}(s,t)$ with s the arc-length variable, the slender-body model is

$$8\pi\mu[\dot{\mathbf{Y}}(s,t)-\mathbf{U}(s,t)] = -\log(e\epsilon^2)\left(\mathbf{I}+\mathbf{Y}_s\mathbf{Y}_s^T\right)\mathbf{F}. \tag{1}$$

Here μ is the surrounding fluid viscosity, $\mathbf{Y}_s$ is tangential to the center-line, $\mathbf{U}(s,t)$ is the fluid velocity at the centerline, $\mathbf{F}$ the force per unit length exerted by the body onto the fluid. ϵ is the slenderness or aspect ratio. The dynamics is asymptotically accurate to $O(\epsilon^2\log\epsilon)$.

Let the object to be a self-propelling rigid rod of length l in a linearized (incompressible) fluid flow $\mathbf{u}(\mathbf{x})$. The rod can be described by its center of mass $\mathbf{X}_c$ and orientation $\mathbf{P}$ as $\mathbf{Y}(s,t) = \mathbf{X}_c(t) + s\mathbf{P}(t)$ for $-l/2 < s < l/2$ and $|\mathbf{P}| = 1$. If the rod has a constant propulsive tangential stress posed on one half of its length and a no-slip condition be imposed on the other half [17], one obtains a basic model for an idealized version of a "pusher" swimmer like a bacterium *E. coli* or a "puller" swimmer like a green algae *C. reinhardtii*. These type of idealized swimmers are extensively used in studies of particle models [33] and are the basis of many continuum theories [34]. A "pusher" swimmer generates the propelling thrust through the trailing flagella, hence in our model the propulsive stress is posed on the lower particle half, as shown in Fig. 1. If the tangential stress is posed on the upper half of the swimmer length, then the particle would an idealized version of a "puller" swimmer, e.g. green algae *C. reinhardtii* which self-propels by pulling its body forth by its front two flagella.

Following the procedure outlined in [17] with zero total force and torque conditions on the swimmer, we can solve for the force $\mathbf{F}(s)$ exerted by the swimmer on the fluid. The swimmer dynamics can be then be encapsulated in the dynamics of its center of mass $\mathbf{X}_c$ and propulsion direction $\mathbf{P}$ as

$$\dot{\mathbf{X}}_c = U_0\mathbf{P} + \mathbf{u}(\mathbf{X}_c), \tag{2}$$

$$\dot{\mathbf{P}} = (\mathbf{I}-\mathbf{P}\mathbf{P}^T)\nabla\mathbf{u}(\mathbf{X}_c)\mathbf{P}. \tag{3}$$

Here U_0 is the constant propulsion speed of the swimmer that depends on the propulsive tangential stress, viscosity, and particle aspect ratio ϵ. The first Eq. (2) describes the dynamics of the center of mass and tells how the particle self-propels and is advected by the fluid flow that is evaluated at the center of mass. The second Eq. (3) is Jeffrey's Equation [21] that describes how a slender rod is rotated by the fluid flow $\mathbf{u}$ evaluated at its center of mass. In our model we non-dimensionalize by the swimmer length and propulsion speed, which sets $l = 1$ and $U_0 = 1$.

If an external flow $\mathbf{v}(\mathbf{x},t)$ is present, then the leading order equations of motion can include it as

$$\dot{\mathbf{X}}_c = U_0\mathbf{P} + \mathbf{u}(\mathbf{X}_c) + \mathbf{v}(\mathbf{X}_c), \tag{4}$$

$$\dot{\mathbf{P}} = (\mathbf{I}-\mathbf{P}\mathbf{P}^T)[\nabla\mathbf{u}(\mathbf{X}_c) + \nabla\mathbf{v}(\mathbf{X}_c)]\mathbf{P}. \tag{5}$$

2.2. Pair interactions

Direct interactions between the micro-swimmers can be included in their dynamics so that they do not overlap or cross. These interactions are commonly referred to as *excluded volume* or *steric*. Borrowing from the field of molecular dynamics, we add short-range repulsive forces between the swimmers via an anisotropic potential by considering the swimmers as soft sphero-cylinders or slender ellipsoidal particles. Commonly used potentials for pair-wise interactions of such anisotropic particles are of the Gay–Berne [13]-type $\Phi^e(\mathbf{r}_{ij},\mathbf{P}_i,\mathbf{P}_j)$ where $\mathbf{r}_{ij} = \mathbf{X}_{ci} - \mathbf{X}_{cj}$ is the distance vector between the two particles' centers of mass and $\mathbf{P}_i$, $\mathbf{P}_j$ their swimming directions. The interaction activates only once the particles are within $2^{1/6} \approx 1.12$ body-lengths away of each-other. The force and torque exerted on the particle i by the particle j are respectively

$$\mathbf{F}^e_{ij} = -\nabla_{\mathbf{r}_{ij}}\Phi^e(\mathbf{r}_{ij},\mathbf{P}_i,\mathbf{P}_j), \tag{6}$$

$$\mathbf{T}^e_{ij} = -\mathbf{P}_i\times\nabla_{\mathbf{P}_i}\Phi^e(\mathbf{r}_{ij},\mathbf{P}_i,\mathbf{P}_j). \tag{7}$$

In this case we consider the pair of particles as force-free and torque-free. By going through the calculation on the previous section (or following the procedure in [17]), but with total force $\mathbf{F}^e_{ij}$ and