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Spontaneous aggregation and global polar ordering in squirmer suspensions ☆

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ABSTRACT

We have developed numerical simulations of three dimensional suspensions of active particles to characterize the capabilities of the hydrodynamic stresses induced by active swimmers to promote global order and emergent structures in active suspensions. We have considered squirmer suspensions embedded in a fluid modeled under a Lattice Boltzmann scheme. We have found that active stresses play a central role to decorrelate the collective motion of squirmers and that contractile squirmers develop significant aggregates.

1. Introduction

Collective motion can be observed at a variety of scales, ranging from herds of large to bacteria colonies or the active motion of organelles inside cells. Despite the long standing interest of the wide implications of collective motion in biology, engineering and medicine (as for example, the ethological implications of the signals exchanged between moving animals, the evolutionary benefits of moving in groups for individuals and for species, the design of robots which can accomplish a cooperative tasks without central control, the understanding of tumor growth or wound healing to mention a few), only recently there has been a growing interest in characterizing such global behavior from a statistical mechanics perspective [1].

Although a variety of ingredients and mechanisms has been reported to describe the signaling and cooperation among individuals which move collectively, it is important to understand the underlying, basic physical principles that can provide simple means of cooperation and can lead to emerging patterns and structures [2]. We want to analyze the capabilities of basic physical ingredients to generate emerging structures in active particles which self propel in an embedding fluid medium. These systems constitute an example of active fluids, systems which generate stresses by the conversion of chemical into mechanical energy. To this end, we will consider model suspensions of swimming particles (building on the squirmer model introduced by Lighthill [3]) and will analyze a hydrodynamically-controlled route to flocking. We will use a hybrid description of an active suspension, which combines the individual dynamics of spherical swimmers with a kinetic model for the solvent. We can identify the emergence of global orientational order and correlate it with the formation of spontaneous structures where squirmers aggregate and form flocks of entities that swim along together. This simplified approach allows us to identify the role of active stresses and self-propulsion to lead both to global orientational order and aggregate formation. Even if in real systems other factors can also control the interaction and collective behaviors of active suspensions, the present description shows that hydrodynamics itself is enough to promote cooperation in these systems which are intrinsically out of equilibrium.

This work is organized as follows. In Section 2.1 we present the theoretical frame of the simulation technique that we have applied, while in Section 2.2 we describe the squirmer model that we have used and introduce the relevant parameters which characterize its hydrodynamic behavior and in Section 2.3 we give a detailed explanation of the simulation parameters and the systems we have studied. Section 3 is devoted to analyze the global polar order parameter and to study quantitatively the orientation that squirmer suspensions display. In Section 4 flocking is studied via generalized radial distribution functions, moreover to characterize the time evolution of the formed flocks, we calculated the time correlation function of the density fluctuations, and the results are shown in this section also. We conclude in Section 5 indicating the main results and their implications.

2. Theoretical model

2.1. Lattice Boltzmann scheme

We consider a model for microswimmer suspensions composed by spherical particles embedded in a fluid. The fluid is modeled using a Lattice Boltzmann approach. Accordingly, the solvent is described in terms of a distribution function $f_i\left(\vec{r};t\right)$ in each node of the lattice. The distribution function evolves at discrete time steps, Δt, following the lattice Boltzmann equation (LBE):

$$f_i\left(\vec{r}+\vec{c}_i\Delta t, t+\Delta t\right)=f_i\left(\vec{r};t\right)+\Omega_{ij}\left(f_j^{eq}\left(\vec{r};t\right)-f_j\left(\vec{r};t\right)\right) \quad (1)$$

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that can be regarded as the space and time discretized analog of the Boltzmann equation. It includes both the streaming to the neighboring nodes, which corresponds to the advection of the fluid due to its own velocity, and the relaxation toward a prescribed equilibrium distribution function f_j^{eq}. This relaxation is determined by the linear collision operator Ω_{ij} [4–6]. It corresponds to linearizing the collision operator of the Boltzmann equation. If Ω_{ij} has one single eigenvalue, the method corresponds to the kinetic model introduced by Bhatnagar–Gross–Crook (BGK) [7]. The LBE satisfies the Navier–Stokes equations at large scales. In all our simulations we use units such that the mass of the nodes, the lattice spacing and the time step Δt are in unity and the viscosity is 1/2, the lattice geometry that we have used was a cubic lattice with 19 allowed velocities, better known as D_3Q_{19} scheme [5].

The linearity and locality of LBE make it a useful method to study the dynamic of fluids under complex geometries, as is the case when dealing with particulate suspensions. Using the distribution function as the central dynamic quantity makes it possible to express the fluid/solid boundary conditions as local rules. Hence, stick boundary conditions can be enforced through bounce-back of the distribution, $f_i\left(\vec{r};t\right)$, on the links joining fluid nodes and lattice nodes inside the shell which defines the solid particles, also known as boundary links [8]. A microswimmer is modeled as a spherical shell larger than the lattice spacing. Following the standard procedure, the microswimmer is represented by the boundary links which define its surface. Accounting for the cumulative bounce back of all boundary links allows to extract the net force and torque acting on the suspended particle [9]. The particle dynamics can then be described individually and particles do not overlap due to a repulsive, short-range interaction among them, given by

$$v^{ss}(r) = \epsilon(\sigma/r)^{\nu_0}, \tag{2}$$

where ϵ is the energy scale, and σ the characteristic width. The steepness of the potential is set by the exponent ν_0. In all cases we have used $\epsilon = 1.0$, $\sigma = 0.5$ and $\nu_0 = 2.0$.

2.2. Squirmer model

We follow the model proposed by Lighthill [3], subsequently improved by Blake [10], for ciliated microorganisms. In this approach, appropriate boundary conditions to the Stokes equation on the surface of the spherical particles (of radius R) are imposed to induce a slip velocity between the fluid and the particles. This slip velocity determines how the particle can displace in the embedding solvent in the absence of a net force or torque. For axisymmetric motion of a spherical swimmer, the radial, v_r and tangential, v_θ components of the slip velocity can be generically expressed as

$$\begin{aligned} v_r|_{r_1=R} &= \sum_{n=0}^{\infty} A_n(t) P_n\left(\frac{\mathbf{e}_1\cdot\mathbf{r}_1}{R}\right), \\ v_\theta|_{r_1=R} &= \sum_{n=0}^{\infty} B_n(t) V_n\left(\frac{\mathbf{e}_1\cdot\mathbf{r}_1}{R}\right), \end{aligned} \tag{3}$$

n-th at the squirmer spherical surface, where P_n stands for the n-th order Legendre polynomial and V_n is define as

$$V_n(\cos\theta) = \frac{2}{n(n+1)}\sin\theta P_n'(\cos\theta), \tag{4}$$

$\mathbf{e}_1$ describes the intrinsic director, which moves rigidly with the particle and determines the direction along which a single squirmer will displace, while $\mathbf{r}_1$ represents the position vector with respect to the squirmer's center, which is always pointing the particle surface and thus $|\mathbf{r}_1| = R$. Since the squirmer is moving in an inertialess media, the velocity $\mathbf{u}$ and pressure p of the fluid are given by the Stokes and continuity equations

$$\nabla p = \nu\nabla^2\mathbf{u}, \quad \nabla\cdot\mathbf{u} = 0. \tag{5}$$

The velocity field generated by the squirmer is the solution of this Eq. (5) under the boundary conditions specified by the slip velocity in the surface of its body, Eq. (3). We will disregard the radial changes of the squirming motion, and will consider $A_n = 0$, to focus on a simple model that captures the relevant hydrodynamic features associated to squirmer swimming. Accordingly, we will also disregard the time dependence of the coefficients B_n and will focus on the mean velocity of a squirmer during a beating period [11]. Hence, from the solution of Eq. (5) using the slip velocity as a boundary condition (Eq. (3)), we can write the mean fluid flow induced by a minimal squirmer as

$$\begin{aligned} \mathbf{u}_1(\mathbf{r}_1) = &-\frac{1}{3}\frac{R^3}{r_1^3}B_1\mathbf{e}_1 + B_1\frac{R^3}{r_1^3}\mathbf{e}_1\cdot\hat{\mathbf{r}}_1\,\hat{\mathbf{r}}_1 - \\ &\frac{R^2}{r_1^2}B_2P_2(\mathbf{e}_1\cdot\hat{\mathbf{r}}_1)\hat{\mathbf{r}}_1, \end{aligned} \tag{6}$$

where we have taken $B_n = 0$, $n > 2$, keeping only the first two terms in the general expression for the slip velocity, Eq. (3). The two non-vanishing terms account for the leading dynamic effects associates to the squirmers. While B_1 determines the squirmer velocity, along $\mathbf{e}_1$, and controls its polarity, B_2 stands for the apolar stresses that are generated by the surface waves [12]. The dimensionless parameter $\beta \equiv B_2/B_1$ quantifies the relative relevance of apolar stresses against squirmer polarity. The sign of β (determined by that of B_2) classifies contractile squirmers (or pullers) with $\beta > 0$ and extensile squirmers (or pushers) when $\beta < 0$. The limiting case when $B_1 = 0$ corresponds to completely apolar squirmers (or shakers [13]) which induce fluid motion around them without self-propulsion. The opposite situation, when $B_2 = 0$ corresponds to completely polar, self-propelling, squirmers which do not generate active stresses around them. We will disregard thermal fluctuations; therefore B_1 and B_2 are the two parameters which completely characterize squirmer motion.

2.3. Simulation details

All the results that we will discuss correspond to numerical simulations consisting of N identical spherical particles in a cubic box of volume L^3 with periodic boundary conditions. In all cases we have considered $N = 2000$, $R = 2.3$ and $L = 100$ (expressed in terms of the lattice spacing). This corresponds to a volume fraction $\phi = 4\pi NR^3/(3L^3) = 1/10$, with a kinematic viscosity of $\nu = 1/2$ (in lattice units) [14]. As we will analyze subsequently, active stresses play a significant role in the structures that squirmers develop when swimming collectively. In Fig. 1 we compare characteristic configurations of suspensions for completely polar, contractile and extensile squirmers. Apolar stresses favor fluctuations in the squirmer concentration and for contractile squirmers there is a clear tendency to form transient, but marked, aggregates. The figure also shows that one needs to distinguish between how squirmers align to swim together and how do they distribute spatially. In the following section we will analyze how active stresses interact with self-propulsion to affect both aspects of collective swimming.