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Large-scale simulation of steady and time-dependent active suspensions with the force-coupling method

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ABSTRACT

We present a new development of the force-coupling method (FCM) to address the accurate simulation of a large number of interacting micro-swimmers. Our approach is based on the squirmer model, which we adapt to the FCM framework, resulting in a method that is suitable for simulating semi-dilute squirmer suspensions. Other effects, such as steric interactions, are considered with our model. We test our method by comparing the velocity field around a single squirmer and the pairwise interactions between two squirmers with exact solutions to the Stokes equations and results given by other numerical methods. We also illustrate our method's ability to describe spheroidal swimmer shapes and biologically-relevant time-dependent swimming gaits. We detail the numerical algorithm used to compute the hydrodynamic coupling between a large collection (10^4–10^5) of micro-swimmers. Using this methodology, we investigate the emergence of polar order in a suspension of squirmers and show that for large domains, both the steady-state polar order parameter and the growth rate of instability are independent of system size. These results demonstrate the effectiveness of our approach to achieve near continuum-level results, allowing for better comparison with experimental measurements while complementing and informing continuum models.

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1. Introduction

Suspensions of active, self-propelled particles arise in both biological systems, such as populations of micro-organisms [1–4] and synthetic, colloidal systems [5]. These suspensions can exhibit the formation of coherent structures and complex flow patterns which may lead to enhanced mixing of chemicals in the surrounding fluid, the alteration of suspension rheology, or, in the biological case, increased nutrient uptake by a population of micro-organisms. In addition to promising applications such as algae biofuels [6,7], characterizing the collective dynamics found in these suspensions is of fundamental importance to understanding zooplankton dynamics [8,9] and mammal fertility [10,11].

The mathematical modeling of active suspensions entails describing how individual swimmers move and interact in response to the flow fields that they generate [12–14]. It is particularly important for these models to be able to handle a large collection of swimmers in order to obtain suspension properties at the lab/*in situ* scale. The modeling of the collec-

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tive behavior of active matter has been a vibrant area of research during the last decade [15,16,14,17], to cite only a few recent reviews. Generally speaking, the modeling approaches can be sorted into two categories: continuum theories and particle-based simulations. Most of the continuum models are generally valid for dilute suspensions where the hydrodynamic disturbances are given by a mean-field description of far-field hydrodynamic interactions [18,19,16]. Recent advances towards more concentrated suspensions include steric interactions [20], but the inclusion of high-order singularities due to particle size remains outstanding. Despite this, these models are very attractive as they naturally provide a description of the dynamics at the population level and the resulting equations can be analyzed using a wide range of analytical and numerical techniques.

Particle-based simulations resolve the dynamics of each individual swimmer and from their positions and orientations, construct a picture of the dynamics of the suspension as a whole. As discussed in [16], particle-based models provide opportunities to (i) test continuum theories, (ii) analyze finite-size effects resulting from a discrete number of swimmers, (iii) explore more complex interactions between swimmers and/or boundaries, and in some cases, (iv) reveal the effects of short-range hydrodynamic interactions and/or steric repulsion. Various models have been proposed in this context, each using different approximations to address the difficult problems of resolving the hydrodynamic interactions and incorporating the geometry of the swimmers. Some of the first such models used point force distributions to create dumbbell-shaped swimmers [21–23], slender-body theory to model a slip velocity along the surfaces of rod-like swimmers [24,25], or the squirmer model [26,27] to examine the interactions between spherical swimmers [28]. These initial studies provided important fundamental results connecting the properties of the individual swimmers to the emergence of collective dynamics. Based on their success, these models have been more recently incorporated into a number of numerical approaches for suspension and fluid-structure interaction simulations including Stokesian dynamics [29–31], the immersed boundary method [32,33], Lattice Boltzmann methods [34,35], and hybrid finite element/penalization schemes [36]. This has allowed for both increased swimmer numbers as well as the incorporation of other effects such as steric interactions, external boundaries, and aligning torques.

In this paper, we introduce an extension of the force coupling method (FCM) [37,38], an approach for the large-scale simulation of passive particles, to capture the many-body interactions between active particles. FCM relies on a regularized, rather than a singular, multipole expansion to account for the hydrodynamic interactions between the particles. It includes a higher-order correction due to particle rigidity by enforcing the constraint of zero-averaged strain rate in the vicinity of each particle. Since the force distributions have been regularized, the total particle force, including that associated with the constraints, can be projected onto a grid over which the fluid flow can be found numerically. This allows the hydrodynamic interactions for all particles to be resolved simultaneously. This mesh can be structured and simple such that an efficient parallel Stokes solver can be used to find the hydrodynamic interactions.

We extend FCM to active particles by introducing the regularized singularities in the FCM multipole expansion that have a direct correspondence to the surface velocity modes of the squirmer model [27]. With these terms included, we then rely on the usual FCM framework to resolve the hydrodynamic interactions in a very efficient manner. We show that by using the full capacity afforded by FCM, we are able to accurately simulate active particle suspensions in the semi-dilute limit with $O(10^4\text{–}10^5)$ swimmers. Using this method, we examine the influence of domain size on the steady-state polar order observed for squirmer suspensions. At the same time, we show that our method is quite versatile, being able to handle time-dependent swimming gaits, ellipsoidal swimmer shapes, and steric interactions, each at a minimal additional computational cost. We explore in detail how to incorporate biologically-relevant, time-dependent swimming gaits by tuning our model to the recent measurements of the oscillatory flow around *Chlamydomonas Rheinardtii* [39]. These experiments revealed that considering time-averaged flows for such micro-organisms may oversimplify the hydrodynamic interactions between neighbors. Time-dependency is also closely associated with the way zooplankton feed, mix the surrounding fluid, and interact with each other [6,9]. As stated in [40], modeling micro-swimmers with a time-dependent swimming gait might be more realistic and should be included in mathematical models and computer simulations. We show that time-dependence can indeed affect the overall organization of the suspension.

We organize our paper as follows: In Section 2, we review FCM and present the theoretical background for its adaptation to active particles. Section 3 details the numerical method, its algorithmic implementation and how the computational work scales with the particle number. In Section 4, we validate the method and test its accuracy by comparing flow fields, trajectories, and pairwise interactions with previous results available in the literature. The effectiveness of our approach is demonstrated in Section 5 where we present results from large-scale simulations of active particle suspensions. Finally, extensions of FCM to more complex scenarios are introduced in Section 6. We simulate suspensions of spheroidal swimmers and demonstrate the new implementation of time-dependent swimming gaits. Here, we also present preliminary results showing the effect of time-dependence on suspension properties.

2. Squirmers using FCM

The force-coupling method (FCM) developed by Maxey and collaborators [37,38] is an effective approach for the large-scale simulation of particulate suspensions, especially for moderately concentrated suspensions at low Reynolds number. In this context, it has been used to address a variety of problems in microfluidics [41], biofluid dynamics [42], and micron-scale locomotion [43–45]. FCM has also been extended to incorporate finite Reynolds number effects [46], thermal fluctuations [47], near contact lubrication hydrodynamics [48,49], and ellipsoidal particle shapes [50]. With these additional features,

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