Simulating active agents with DPD hydrodynamics

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In this ongoing work we are developing a framework to simulate active agents taking into account both hydrodynamics and thermal fluctuations. Currently we are limiting our study to colloids and polymers although the framework will be applicable to agents with a wide range of structures. To achieve this we propose an extension of the widely known simulation software LAMMPS [1] that allows the implementation of hydrodynamic self-propulsion via force redistribution among solvent particles, this extension, in combination with the Dissipative Particle Dynamics (DPD) package [2], enables these kind of simulations.

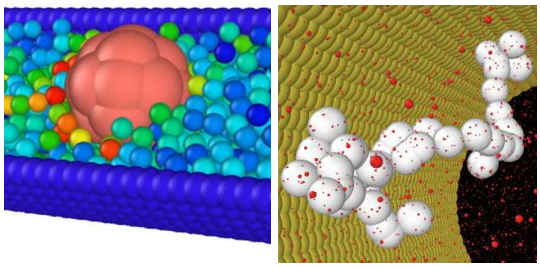

Fig. 1. Active colloid (left) and polymer (right) inside a channel full of DPD solvent.

Similar approaches using lattice Boltzmann (LB) methods [3] and Multi-Particle Collision dynamics (MPC) [4] have been already well studied. With DPD and MPC dynamics we can easily simulate agents with more complex shapes taking into account thermal fluctuations, both of which are harder to implement using LB methods. Our approach takes advantage of the versatility of the LAMMPS code, being MPI-parallelizable and allowing the combination of our implementation with the wide range of features LAMMPS offers.

We are interested in the subsets of active matter systems known as active colloids [5, 6] and active polymers [7], which have very useful and broad applications [8]. Their collective behaviour is rich and complex, and in many cases cannot be ascribed solely to the agents motion: hydrodynamic interactions need to be taken into account [9]. This is the case, for example, of many self-propelled microorganisms, or *microswimmers* [10], whose movement is an essential aspect of life. A successful model for this systems is the so-called *squirmer* [11, 12], in their simplest form these are hard spheres that take into account the propulsion induced by the beating cilia and flagella as a prescribed steady velocity of the solvent particles tangential to the surface of the sphere. This model serves as inspiration for our project.

The equations of motion of our model for the agent (i) and the solvent particles (j) read,

$$\boldsymbol{F}_i = \boldsymbol{F}_i^{\mathrm{DPD}} + \boldsymbol{F}_i^{T} \quad \text{and} \quad \boldsymbol{F}_j = \boldsymbol{F}_j^{\mathrm{DPD}} + \boldsymbol{F}_j^{H} \qquad (1)$$

where $\boldsymbol{F}^{\mathrm{DPD}} = \boldsymbol{F}^{C} + \boldsymbol{F}^{D} + \boldsymbol{F}^{R}$ represent respectively the conservative, dissipative and random forces of the DPD interaction, $\boldsymbol{F}^{T}$ corresponds to the thrust exerted by the agents propulsion, which causes a hydrodynamic reaction force, $\boldsymbol{F}^{H}$, on the solvent particles. This hydrodynamic force field results from the two first angular modes B_1 and B_2 of the surface velocity field of the squirmer model. The first mode determines the maximum velocity the swimmer can achieve, while their ratio $\beta = B_2/B_1$ captures different types of swimmers which perturb their surrounding fluid in different ways, pushers ($\beta < 0$), pullers ($\beta > 0$), neutrals ($\beta = 0$) and shakers ($\beta \to \infty$).

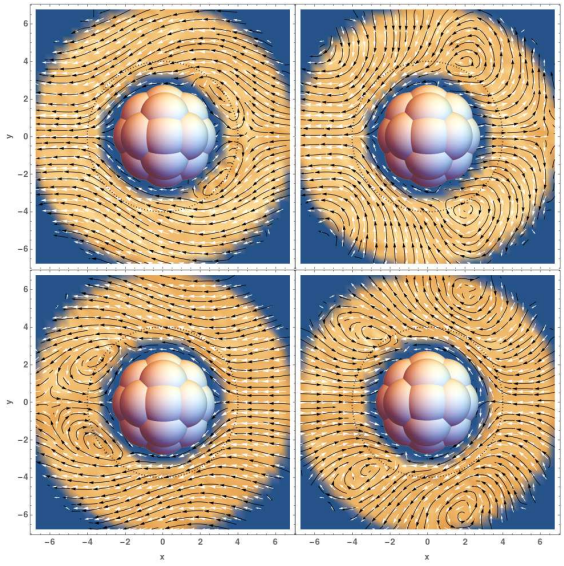

Fig. 2. Solvent velocity field around a squirmer self-propelling in the positive x-axis in the colloid (left) and laboratory (right) reference frame, for $\beta = -5$ (*pusher*, top) and $\beta = 5$ (*puller*, bottom).

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