Internship: an efficient computational framework to study collective motion in reactive suspensions.

Supervisors: Blaise Delmotte[1] and Sebastien Michelin[2]

[1] blaise.delmotte@ladhyx.polytechnique.fr,
[2] sebastien.michelin@ladhyx.polytechnique.fr

We have all witnessed the flocking of starlings in the sky and the schools of fish that form in the ocean. This kind of organization of living systems is not limited to those that we see, but also occurs for those that we don't: swimming micro-organisms. Suspensions of micro-swimmers, such bacteria or sperm cells, exhibit a rich dynamics. They can form coherent structures due to collective motion, mix the surrounding fluid or modify its rheological properties. More recently, artificial micro-swimmers have been developed to mimic these behaviors, but also to achieve specific functions, such as targeted drug delivery or transport in microfluidic systems. In particular, phoretic micro-swimmers have recently received much attention. These particles react with the surrounding solvent and interact with their neighbors (Fig 1a). The motion of large collections of phoretic particles remains to be explored because of the complex interplay between chemical reactions and hydrodynamic interactions. In this sense, numerical methods offer a promising tool. Yet, including an accurate description of the micro-swimmers in a suspension containing thousands (or millions) individuals, requires considering a wide range of coupled scales (from one micron, 10^{-6}m, to several millimeters, 10^{-3}m). What happens at large scales depends on sophisticated mechanisms occurring two or three orders of magnitude below. Therefore, efficient numerical methods are needed to simulate such systems at the macroscopic scale, while keeping an accurate description at the individual level.

The goal of this internship is to extend a well-known numerical method used to simulate particle suspensions: the Force Coupling Method (FCM). FCM has already been used to simulate suspensions of magnetic particles and micro-swimmers at very large scales (cf. Fig 1b), but reaction with the solvent still remains to be included. The intern will first review the litterature on reactive particles and numerical methods for particle suspensions. She/he will then develop a simple code to solve the Laplace equations for the reactant concentration and validate it with existing solutions. After validation, the tool will be included in an existing code that already solves the fluid phase. Eventually, she/he will simulate suspensions at large scale and characterize the various collective states that emerge.

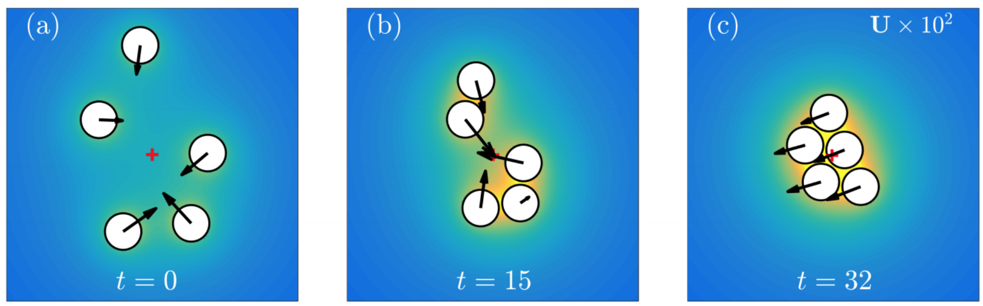
Prospective candidates must have a solid background in Microhydrodynamics, Computational Fluid Dynamics and Programming.

This internship will be held at LadHyX (Ecole Polytechnique) and may be followed by a Ph.D. depending on the progress of the candidate.

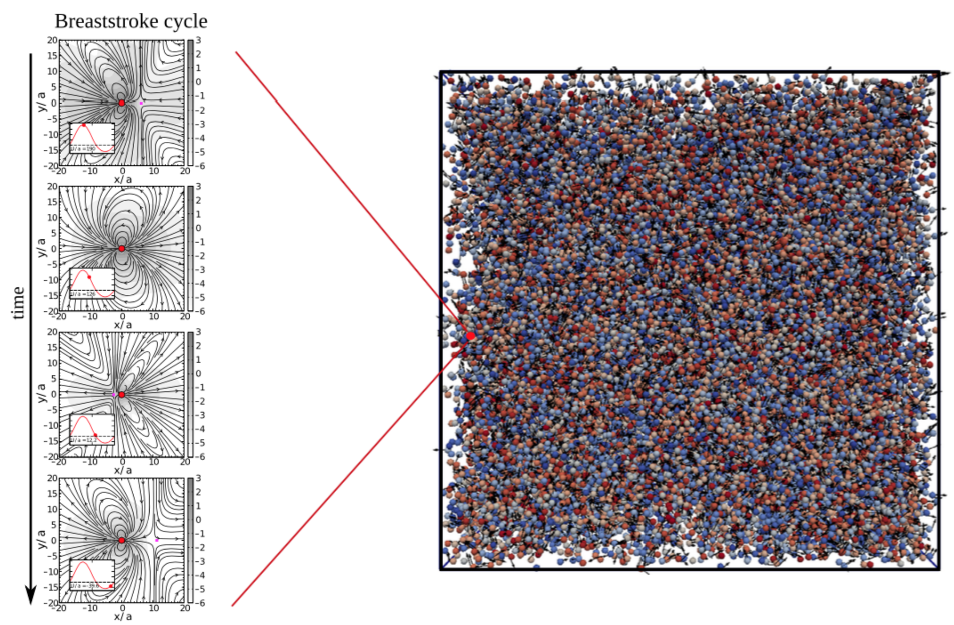
References

[1] Akhil Varma, Thomas D. Montenegro-Johnson, and Sebastien Michelin. Clustering-induced self-propulsion of isotropic autophoretic particles. *Soft Matter*, 14:7155–7173, 2018.

[2] Blaise Delmotte, Eric Keaveny, Franck Plouraboue, and Eric Climent. Large-scale simulation of steady and time-dependent active suspensions with the force-coupling method. *Journal of Computational Physics*, 2015.



(a) Clustering of phoretic micro-swimmers due to the coupling between chemical reactions and hydrodynamic interactions [1].



(b) Simulation of 40000 breast-stroke micro-swimmers immersed in a viscous fluid using the Force Coupling Method (FCM) [2].

Figure 1