Coarse-graining computation of collective swimming in biosuspensions.

Project: Coarse-graining techniques for modeling highly heterogeneous complex biomaterials

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Abstract

Bacteria are the most abundant organisms on Earth and they significantly influence carbon cycling and sequestration, decomposition of biomass, and transformation of contaminants in the environment. Therefore, an understanding of the basic principles of bacterial behavior and its control is of natural importance to the DOE mission. Our analytical, numerical and experimental studies reveal that swimming of bacteria drastically alters the material properties of the bacterial suspension: the experiments indicate a 7-fold reduction of the effective viscosity and a 10-fold increase of the effective diffusivity of the oxygen and other constituents of the suspending fluid. The principal mechanism behind these unique macroscopic properties is self-organization of the bacteria at the microscopic level – a multiscale phenomenon. Understanding the mechanism of self-organization in general is a fundamental issue in the study of biological systems. Our work in this area includes

- *Numerical modeling.* Bacteria are modeled as self-propelled point force dipoles subject to two types of forces: hydrodynamic interactions with the surrounding fluid and excluded volume interactions with other bacteria modeled by a Lennard-Jones-type potential. This model, allowing for numerical simulations of a large number of particles, is implemented on the Graphical Processing Units (GPU), and is in agreement with experiments.

- *Study of Dilute suspensions.* An explicit asymptotic formula for the effective viscosity in terms of known physical parameters is derived. This formula is then compared with that derived for a dilute suspension of prolate spheroids driven by a stochastic torque, which models the "tumbling" behavior – the random reorientation of bacteria. It is shown that the steady-state probability distributions of single particle configurations are identical for the dilute and semi-dilute models in the limiting case of particles becoming spheres. Thus, a deterministic system incorporating pairwise hydrodynamic interactions and excluded volume constraints behaves as a system with a random stochastic torque. This phenomenon of stochasticity arising from a deterministic system is referred to as *self-induced noise.*

- *Kinetic collisional model.* Most of the previous work on bacterial suspensions ignores collisions. These inelastic interactions lead to an alignment of the nearby-swimming bacteria, which has been indeed observed experimentally. To understand the onset of collective motion in the above model, we investigate the correlation of bacterial velocities and orientations as a function of the interparticle distance. We seek to capture a second order phase transition in the bacterial suspension – an gradual appearance of correlations and local preferential alignment with an increase of concentration. A probabilistic model for the distribution function for bacterial positions and orientations will be derived in the presence of self-induced noise (work in progress).

- *PDEs with many non-separated scales and irregular coefficients:* Classical FEM and homogenization do not work. Designed shape functions that capture scales (with H.Owhadi).

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