The packaging and transport of cholesterol in the bloodstream are mediated by nanoparticles called lipoproteins. The functional properties of HDL are thought to be closely tied to shape. A discoidal HDL particle consists of an open lipid bilayer bound by an apolipoprotein apo A-I chain. Motivated by experimental and numerical studies revealing that discoidal high-density lipoprotein (HDL) particles may adopt flat elliptical and nonplanar saddle-like configurations, a variational description is developed to explore the stability of a flat circular discoidal HDL particle. While the lipid bilayer is modeled as a two-dimensional fluid film endowed with surface tension and bending elasticity, the apo A-I chain is modeled as a one-dimensional inextensible twist-free rod endowed with bending elasticity. Stability is investigated using the second variation of the energy functional. Various planar and nonplanar instability modes are predicted and corresponding critical values of the salient dimensionless parameters are obtained. Results predict that the first planar and nonplanar unstable modes occur due to in-plane elliptical and transverse saddle-like perturbations. Using available data, detailed stability diagrams indicate the range of input parameters for which a flat circular discoidal HDL particle is linearly stable or unstable.
The classical slender-body theory for viscous flows was initiated by Burgers in 1938 and was developed in the seventies with the primary objective of obtaining the drag force and torque required to sustain the rigid motion of slender bodies in viscous fluids. One important goal of this effort was to provide estimates for parameters such as the effective viscosity of suspensions of solid particles in fluids. Despite the success in describing the viscous flow generated by a single particle of general shape, the treatment of a more realistic number of suspended particles represents a formidable computational challenge. Our approach to slender-body theory, which aims to reduce the computational complexity of the problem, involves replacing slender three-dimensional particles with lower-dimensional objects and the surrounding Newtonian fluid by a quasi-Newtonian second-gradient fluid. In such a fluid, an additional parameter, namely the product of the viscosity and a characteristic length—called the gradient length—enters the flow equation, which resembles the well-known hyperviscous regularization of the Navier–Stokes equation. The central idea underlying our approach is that the aforementioned gradient length represents the effective thickness of the lower-dimensional objects, in the sense that the drag force and torque required to sustain their rigid motion in a hyperviscous fluid are the same as those required to sustain the corresponding motion of a particle with thickness coincident with the gradient length in a Newtonian fluid. Importantly, both the dimensional reduction and the hyperviscous regularization, combined with suitable numerical schemes, can be used also in situations where inertia is not negligible.
A simple model for simulating flows of active suspensions is presented. The approach is based on the dissipative particle dynamics framework. While the model is potentially applicable to a wide range of self-propelled particle systems, the specific class of self-motile bacterial suspensions is considered as a modeling scenario. To mimic the rod-like geometry of a bacterium, two dissipative particle dynamics particles are connected by a stiff harmonic spring to form an aggregate dissipative particle dynamics molecule. The bacterial motility is modeled through a constant self-propulsion force applied along the rod axis of each such aggregate molecule. The model accounts for hydrodynamic interaction forces between self-propelled agents through the pairwise dissipative interaction forces from the dissipative particle dynamics framework. Numerical simulations of this system are performed using a customized version of the open-source LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) software package. Detailed studies of the influence of particle concentration, pairwise dissipative interaction forces, and Stokes drag forces on the statistics of the system are provided.