Statistical mechanics for complex, multiphase fluids

Complex, multiphase fluids have wide-ranging applications in physics, engineering and biology. For some such systems, e.g. atomic and molecular fluids, the dynamics are well-described by continuum models, such as the Navier-Stokes equations. In contrast, and of particular interest in this talk, are colloidal fluids, which consist of a large number of nano- to micro-metre size particles, suspended in a bath of many more, much smaller and much lighter particles. Common everyday examples are paints, inks, blood and milk. Such fluids exhibit interesting and non-trivial dynamics on lengthscales from the particle size up to the macroscale, and as such are out of reach of continuum models. Additionally, the large number of particles leads to high-dimensional models that are computationally intractable, and there is thus the need for systematically derived, accurate and efficient reduced models.

In recent years, a number of dynamic density functional theories (DDFTs) have been developed to describe colloidal dynamics. These DDFTs aim to overcome the high-dimensionality by reducing to the dynamics of the one-body density, described by a (integro-)PDE in only three spatial dimensions, independently of the number of particles. We focus particularly on the inclusion of inertia and hydrodynamic interactions, both of which strongly influence non-equilibrium properties of the system. We derive a general DDFT, the results of which are in very good agree ment with the full underlying Langevin dynamics. We also show that, in suitable limits, many existing DDFTs are special cases of our formulation, and that close to local equilibrium we obtain a Navier-Stokes-like equation with additional non-local terms. Finally, we describe the rigorous passage to the high-friction limit, where the one-body density satisfies a nonlinear, non-local Smoluchowski-like equation with a novel diffusion tensor.

Joint work with Serafim Kalliadasis, Andreas Nold and Greg Pavliotis.