Particle-based hydrodynamics

with Ellák Somfai (Physics and Complexity)
E.Somfai@warwick.ac.uk

Numerical methods simulating hydrodynamics with finite difference or finite volume methods have a long established tradition in science and engineering. Independently, there is a number of alternative methods emerging, including dissipative particle dynamics (DPD), stochastic rotation dynamics (SRD), smooth particle hydrodynamics (SPH), lattice-Boltzmann methods, etc. In many of these methods (eg. the first three in the list above) hydrodynamics is simulated by tracking the motion of a large number of interacting particles, which can be considered as "patches of fluid". While these methods are less mature, they offer a number of advantages over conventional methods. Among these are the natural inclusion of fluctuations, which are important for mesoscopic systems; it is relatively easy to implement complex boundary conditions, eg. simulating flow in porous media; as well as a number of these methods are flexible to simulate non-trivial fluids: multi-phase flow, non-Newtonian fluids (polymer solutions and melts), etc.

The goal of this miniproject is to assess and improve the performance of some of these particle-based hydrodynamics methods for potential applications. One major issue is compressibility: particle-based methods typically simulate very compressible fluids, while applications often require incompressible flow. The primary target will be to address the compressibility for DPD and SRD. Further potential problems include boundary conditions, eg. addressing the non-physical layering effect found in some of the particle-based methods, coupling flow to elastic boundary conditions etc.

The work is numerically oriented and involves significant amount of programming. While it is always encouraged to write own code for scientific research, due to the timeframe of the miniproject, working code for DPD and code fragment for SRD will be available.

This miniproject has prospects to evolve into a PhD project. This could involve collaboration with Warwick Engineering and Warwick Medical School on the simulation of blood flow in capillaries, where the red blood cells are modelled as immersed elastic bodies.