UAMMD: Complex fluids in the GPU era

Raul P. Pelaez[1], and Rafael Delgado-Buscalioni[1]
[1]Departamento de Fsica Terica de la Materia Condensada, Universidad Autnoma de Madrid.

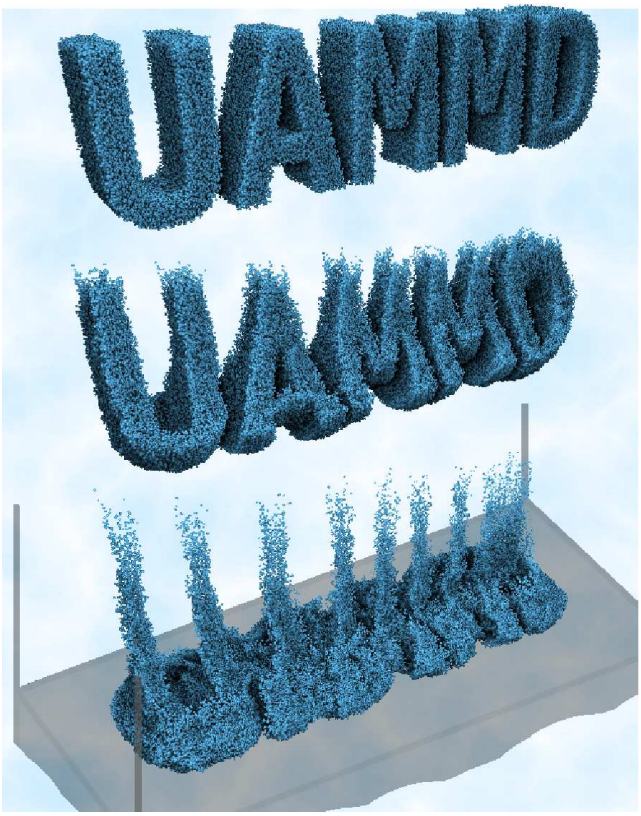

Figure 1: UAMMD logo made up of 10^6 particles sedimenting under a gravity field in a low Reynolds flow.

Complex fluids is an umbrella where solute particles and liquid phase coexist, embracing inorganic and organic soft matter, nanoparticles, polymers, colloids, membranes, interfaces, and hydrodynamics at different spatio-temporal regimes. To face this challenge, we present the "Universally Adaptable Multiscale Molecular Dynamics" code (UAMMD) [1], a novel, open-source, massive parallel, software infrastructure for soft matter simulations in Graphical Procesor Units (GPU). Starting from few nanometers up, UAMMD allows for Lagrangian simulations (MD, DPD, SPH, Brownian hydrodynamics, etc.) and also hybrid Eulerian-Lagrangian schemes.

One of the strongholds of UAMMD is to couple continuum fields with particles. Using the immersed-boundary formalism, Landau-Lifshitz fluctuating hydrodynamics are coupled to MD and this idea is generalized to other fields to model opto-hydrodynamics, charge dynamics, magnetic nanoparticles, etc. UAMMD naturally embraces coarse-grained models of proteins and any other tailored model. I will introduce UAMMD and expose my attempts to push the boundaries of numerical simulation of complex fluids, revisiting old and new schemes in the eyes of a GPU.

---

[1] |https://github.com/RaulPPelaez/UAMMD|