INVITED SESSION

Multiscale modelling of complex fluids using particle-based methods

ORGANIZERS

Nicolas Moreno*, Florencio Balboa Usabiaga*, Marco Ellero*

***** BCAM - Basque Center for Applied Mathematics, Mazarredo 14, E48009 Bilbao, Spain

Keywords: Particle-based methods, rheology, mesoscopic flows, Brownian motion, active matter.

ABSTRACT

Computational fluid dynamics has traditionally preferred Eulerian discretizations of the underlying partial differential equations (PDE) to model flows. This approach has been used to simulate not only the Navier-Stokes equation but also PDEs for non-Newtonian fluids and their extensions to fluctuating hydrodynamics. Despite their strengths, Eulerian discretizations have also some drawbacks. As the methods are extended to model complex suspensions at mesoscopic scales it is often necessary to make assumptions about the constitutive equations of state or the nature of the transport coefficients using phenomenological approximations. They typically enforce spatial/temporal scales separation that apply only at macroscales, and are unable to capture complex history-dependent flows. Additionally, it is challenging to treat complex geometries, especially moving boundary conditions, and it can be difficult to couple the macroscopic variables to microscopic ones.

One possibility to overcome these challenges is to use particle-based methods and hybrid schemes. These approaches have some advantages that made them quite versatile to study mesoscopic flows. Particle-based methods are flexible, they can introduce easily new models to simulate complex fluids, they can deal with complex boundary conditions and immersed moving particles, and over the last twenty years we have learnt how to include thermal fluctuations consistent with thermodynamics. They are also well suited to include physical properties derived from coarse-grained techniques.

The focus of this mini-symposium is bring together state of the art particle-based methods to model complex flows (i.e. colloidal/non-colloidal suspensions of complex shaped objects, emulsions, multiphase flows, polymeric systems, active matter, etc.) at mesoscales, as well as hybrid methodologies for multiscale modelling. Some methods relevant for this mini-symposium are Coarse-Graining Molecular Dynamics (CG-MD), Dissipative Particle Dynamics (DPD), Smoothed Dissipative Particle Dynamics (SDPD), Smoothed Particle Hydrodynamics (SPH), Moving Particle Semi-Implicit Method (MPS), Brownian Dynamics (BD) or Stokesian Dynamics (SD). Applications that showcase the power of these methods or multiscale-hybrid schemes to study the rheology and dynamics of complex fluids are welcome.