14th World Congress on Computational Mechanics (WCCM XIV)
8th European Congress on Computational Methods in Applied Science and Engineering (ECCOMAS 2020)
July 19- 24, 2020, Paris, France

PARTICLE-BASED METHODS FOR THE SIMULATION OF COMPLEX FLUIDS

TRACK NUMBER (600-700)

M. ELLERO* AND D. FEDOSOV†

* Basque Center for Applied Mathematics
Alameda de Mazarredo 14, 48400 Bilbao, Spain
Email: mellero@bcamath.org

† Institute of Complex Systems (ICS-2)
Research Center Juelich, Germany
Email: d.fedosov@fz-juelich.de

Key words: particle-based methods, mesoscopic flows, complex fluids, microfluidics, rheology, non-Newtonian fluid mechanics, fluctuating hydrodynamics.

ABSTRACT

In the area of complex fluid modelling and simulations, traditional methods based on homogenization and discretization of partial differential equations (PDE), i.e. using grid-based techniques such as finite elements, finite volumes or finite differences methods, have been the main driver of computational research in the past decades and have helped to elucidate several problems in rheology and non-Newtonian fluid mechanics. Although being very successful, PDE-based approaches typically enforce spatial/temporal scales separation and are valid only on macroscopic scales. Moreover strong physical assumptions are required to close the PDEs, producing constitutive equations which are approximate in many cases.

In recent years, there has been an increasing interest in simulating complex fluids starting from consistent mesoscopic and micro-structural models and reproducing the complex macroscopic flow behavior as a bottom-up approach, rather than relying on continuum PDE.

Numerical methods amenable for this specific modelling approach need to embed several features, i.e. (i) they must be able to model consistently Brownian motion and fluctuating hydrodynamics crucial at the mesoscopic scales; (ii) complex physics should be incorporated easily in the algorithmic structure; and (iii) they need to be robust and highly scalable, the last feature being crucial to reach the relevant macroscopic spatial and temporal scales required in experiments.

Particle methods meet these requirements and they are becoming increasingly popular in the complex fluid modelling community. The objective of this symposium is to bring international scientists together working in the area of particle-based modelling of complex fluids. Numerical methods include but are not restricted to Coarse-Graining Molecular Dynamics (CG-MD), Dissipative Particle Dynamics (DPD), Smoothed Dissipative Particle Dynamics (SDPD), Smoothed Particle Hydrodynamics (SPH), Lattice-Boltzmann Method

(LBM), Moving Particle Semi-Implicit Method (MPS), Brownian Dynamics (BD) or Stokesian Dynamics (SD).

Focus of the mini-symposium will be on the modelling of the dynamics and the rheology of complex fluids, i.e. colloidal/non-colloidal suspensions of rigid particles or cells/vesicles, emulsions, multiphase flows, polymeric systems, mixtures, shear-induced particle migration, particle separation, mixing, microfluidics etc. The goal is, on one hand, to share state-of-the-art results on rheology and dynamics of complex fluids and, on the other to discuss technical issues on their computational modelling. We believe that this mini-symposium will foster new collaborations and contribute to further advances in the field.