A PARTICLE BASED PLATFORM FOR FLOW SIMULATION WITH MAGNETIC AND OTHER DEGREES OF FREEDOM

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We review our work on particle based fluid dynamic simulations with macroscopic as well as mesoscopic methods. Macroscopically, a versatile alternative to grid-based discretisations of the equations of continuum mechanics, such as the Navier Stokes equations in fluid dynamics, are Lagrangian particle based methods, for example Smoothed particle hydrodynamics (SPH) [1]. On a mesoscopic scale, where thermal fluctuations start to play a role, Dissipative particle dynamics (DPD) [2] can be used. All our applications of these methods, as well as the Molecular dynamics method for atomistic simulations, have been performed on the common simulation platform SYMPLER [3]. A unique feature of SYMPLER is the possibility to assign arbitrary additional internal degrees of freedom to the fluid particles, together with user-defined material models and dynamic evolution equations. This feature allowed us to tackle fluid-dynamic problems from various fields from which we will highlight a few: In the field of process engineering, we simulated micro powder injection moulding (micro-PIM) of powder filled feedstocks, and micro-casting of metal alloys for ceramic and metallic micro-parts. Special aspects that have been investigated in detail for micro-PIM are yield-stress and shear thinning effects [4, 5] and their interplay with powder segregation in the feedstock [6, 7]. We found a significant influence of the flow profile on the local solids concentration and also in return, of the local rheology on the filling pattern. The dynamics of the solid fraction in particular was incorporated into the fluid dynamics by a discretisation of Phillips’ model for shear induced migration [8] on SPH-fluid particles. While in the original application the model was parametrised by means of MRI concentration measurements for dense suspensions, we had to rely for now on an a-posteriori-analysis of the solid micro-parts with highly energetic X-rays [7]. On the other hand we have also been able to directly connect particle
based flow simulation to MRI-experiments: We performed constraint SPH-simulations of haemodynamics for the estimation of blood flow measurements with magnetic resonance imaging [9]. Additionally, by making direct use of the mentioned flexibility in assigning additional degrees of freedom to the fluid particles, we have directly coupled hydrodynamic convective transport and the dynamics of local magnetisations within the framework of the Bloch equations [10]. By applying the DPD-method, this allows to directly simulate the MRI-measurement of the fluid’s self-diffusion due to the thermal fluctuations in order to assist the design of better MRI-experiments.

REFERENCES


