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COLLOQUIUM

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Particle based hydrodynamics and flow simulations on massively parallel computers

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Mesoscale simulations of hydrodynamic media have attracted great interest during the last years in order to bridge the gap between microscopic simulations on the atomistic level on the one side and macroscopic calculations on the continuum level on the other side. Various methods have been proposed which all have in common that they solve the Navier-Stokes equations in different types of discretizations, e.g. Lattice-Boltzmann simulations on a spatial grid. Grid-free methods are mainly based on the concept of particles and include methods like Dissipative Particle Dynamics (DPD) or Multi-Particle Collision Dynamics (MPC). In the latter approach, pseudo-particles are considered to carry both hydrodynamic information and thermal noise. With a small set of parameters (particle density, scattering angle, mean free path of a particle) it is possible to reproduce hydrodynamic behavior. In particular, the regime of small Reynolds numbers has been investigated in detail, e.g. Poiseuille flow, shear flow, vortices or hydrodynamic long time tails, to name a few.

In the present talk some recent developments in Multi-Particle Collision Dynamics are presented, including a scalable implementation (MP2C) for massively parallel computers. The program enables a coupling between molecular dynamics simulations and a mesoscopic solvent, and therefore takes into account hydrodynamic interactions between solutes. For dilute systems of solutes, load balancing issues are discussed. Furthermore, an implementation of a local thermostat is presented which takes into account statistical fluctuations in energy distributions of small set of particles and therefore enables a local temperature control of systems under non-equilibrium conditions. A recently developed theoretical description enables the proper treatment of a thermostat into dynamical quantities, like dynamic structure factors. Examples are shown for semi-dilute polymer solutions in shear flow as well as Poiseuille flow simulations as well as recent results for low Reynolds flow through stochastic geometries, representing the gas diffusion layer of fuel cell systems. Boundary conditions on surfaces can be modeled from slip to no-slip boundary conditions taking into account hydrophillic and hydrophobic effects of surfaces.