



ICAMS Special Seminar

Friday, 05 February 2016, 2.30 – 3.30 p.m.
Room IC 02-158/88

Dr. Godehard Sutmann

Institute of Advanced Simulations (IAS), Jülich Supercomputing Centre (JSC)
Forschungszentrum Jülich, Germany
{g.sutmann}@fz-juelich.de

2.30 – 3.10 p.m. Research Presentation

Including hydrodynamics and adaptivity in particle systems on parallel computers

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 and macroscopic calculations on the continuum level. 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.

In the present talk some recent developments in the mesh-free method, Multi-Particle Collision Dynamics, are presented, including a scalable implementation (MP2C) for massively parallel computers. The method enables a coupling between molecular dynamics simulations and a mesoscopic fluid, taking into account hydrodynamic interactions between atomistic particles. For dilute systems of solutes, load balancing issues are discussed and a dual domain decomposition approach is presented. Furthermore, a scheme of a local thermostat is presented, which takes into account statistical fluctuations in energy distributions of small sets of particles and therefore enables a local temperature control of systems under non-equilibrium conditions. Applications are shown for, e.g. semi-dilute polymer solutions in shear flow or simulations of flow in stochastic geometries of a gas diffusion layer. As an extension to the one-level approach, a hybrid scheme is presented which allows a change in resolution between a mesoscopic and atomistic description of the fluid leading to an adaptive description of solvent properties.

3:10 – 3:30 p.m. Lecture

Introduction to non-linear optimization problems