Multi-Particle Collision Dynamics coupled to Molecular Dynamics 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 mircoscopic 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[1,2] on a spatial grid or Multi-Particle Collision Dynamics (MPC) — also called Stochastic Rotation Dynamics (SRD) — using discrete particles[3,4]. 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[4,5].

One advantage of the MPC method is that a coupling to atomistic simulations can be established in a simple way. The main characteristic of MPC is that particles are sorted into the cubic cells (with lattice constant a) of a randomly positioned collision grid. Different variants of MPC vary in the way how the momentum exchange between particles within a collision cell is performed. In the SRD-version of MPC, relative velocities are rotated randomly by a given angle around a randomly chosen direction, which mimics collisions between solvent molecules. If coupled to atomistic simulations of solute particles, e.g. by molecular dynamics (MD), the MD-particles are sorted together with fluid particles into collision cells and their velocities are included into the stochastic rotation step. Because atomistic time scales are typically smaller than hydrodynamic time scales, MD-particles are basically simulated according to their force-fields. In order to establish a coupling to the hydrodynamic medium, they are included every n-th step into a stochastic rotation together with the solvent particles.

Since in typical simuations of colloidal suspensions or semi-diluted polymer systems, fluid particles are $1-5$ orders of magnitude more numerous than MD-particles, system sizes get very large in simulations of $10^4 - 10^6$ MD-particles. Therefore, although mesoscale hydrodynamics techniques are algorithmically simple, the computational demand to study large system sizes on long time scales requires an efficient parallel implementation of the simulation code.

In the present work, a highly scalable implementation of the MPC algorithm, coupled to

MD is presented[6]. The current version uses a domain decomposition approach, based on MPI. For the SRD part communication between processors is basically reduced to nearest neighbor exchange of collision cell information. The MD part is implemted via an eigth shell (ES) communication for the force computation and a minimum transfer scheme for the particle export/import. It is demonstrated that the program scales for the SRD part to the full capacity of the BlueGene/P architecture at JSC, i.e. 65536 compute cores. This particle based multiscale implementation, including various types of boundary conditions, offers the large scale simulation of microscopic systems coupled to a mesoscopic flow model on extended time scales.

References

1. S. Succi. *The Lattice Boltzmann Equation: For Fluid Dynamics and Beyond*. Oxfor University Press, Oxford, 2001.
2. B. Dünweg and A.J.C. Ladd. Lattice Boltzmann Simulations of Soft Matter Systems. *Adv. Polym. Sci.*, 221:89–166, 2009.
3. A. Malevanets and R. Kapral. Mesoscopic model for solvent dynamics. *J. Chem. Phys.*, 110:8605–8613, 1999.
4. G. Gompper, T. Ihle, D.M. Kroll, and R.G. Winkler. Multi-Particle Collision Dynamics: A Particle-Based Mesoscale Simulation Approach to the Hydrodynamics of Complex Fluids. *Adv. Polym. Sci.*, 221:1–87, 2009.
5. R. Kapral. Multiparticle Collision Dynamics: Simulation of Complex Systems on Mesoscales. In S.A. Rice, editor, *Adv. Chem. Phys.*, volume 140, page 89. Wiley, 2008.
6. G. Sutmann, R. Winkler, and G. Gompper. Multi-particle collision dynamics coupled to molecular dynamics on massively parallel computers. (in preparation), 2009.