Massively Parallel Molecular-Continuum Simulations with the Macro-Micro-Coupling Tool

Overview
Efficient implementations of hybrid molecular-continuum flow solvers are required to allow for fast and massively parallel simulations of large complex systems. Several coupling strategies have been proposed over the last years for 2D/3D, time-dependent/ steady-state or compressible/incompressible scenarios. Despite their different application areas, most of these schemes comprise the same or similar building blocks. Still, to the authors’ knowledge, no common implementation of these building blocks is available yet. In this contribution, the Macro-Micro-Coupling Tool is presented which is meant to support developers in coupling mesh-based methods with molecular dynamics. It is written in C++ and supports two- and three-dimensional scenarios. Its design is reviewed, and aspects for massively parallel coupled scenarios are addressed. Scaling results are presented for a hybrid simulation which couples a molecular dynamics code to the Lattice Boltzmann application of the Peco framework.

MaMiCo: Macro-Micro-Coupling Tool

- C++-development for spatiotemporal hybrid molecular-continuum simulations
- Support of 2D/3D hybrid scenarios
- Macroscopic cells within MaMiCo are used to
  - map macroscopic quantities between the macroscopic solver and MaMiCo
  - map macro/microscopic quantities between the MD solver and MaMiCo
- Particle insertion/deletion [2] encapsulated within MaMiCo

Parallel Results
- Channel flow simulation with MD region embedded in the center
- LB solver: sequential, 54 × 54 × 54 cells, BGK
- MD solver: parallel, 1 000 000 single-centered LJ molecules
- LB – MD: Velocity relaxation in (MD) boundary cells, retaining mass in outermost cells using USHER
- MD – LB: Only map velocities and incorporate them into particle distribution functions

Outlook: Nanofilters
- Flow between two reservoirs through a molecular filter
- Flow simulation in reservoirs: LB
- Simulation of flow through filter: MD
- Fully three-dimensional steady-state coupling based on [3]

Macroscopic Cell Exchange
- MPI-based exchange of macroscopic cell information between MD and LB
- Exchange (mostly) hidden from user
- Example: LB on one process, MD on four processes

References