Master Project: Coupling ESPResSo++ and MaMiCo

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Hybrid molecular-continuum methods enable the multiscale simulation of complex fluid flow: the computational domain is divided into a continuum and a molecular dynamics (MD) subdomain. The MD domain is typically rather small, and the flow inside this domain is determined by simulating individual molecules. The continuum domain is treated by a continuum method, such as a mesh-based Navier-Stokes solver. Over the last years, the macro-micro-coupling tool (MaMiCo) evolved and can be used to plug together arbitrary continuum and MD solvers. MaMiCo can be run on clusters (MPI support) and already interfaces various software packages, including LAMMPS, ls1 mardyn and ESPResSo (on MD side) and waLBerla, Palabos and OpenLB (on mesh-based solver side).
In this project, MaMiCo interfaces shall be implemented for the ESPResSo++ framework. This framework is special in the sense that it implements the adaptive resolution scheme — a method which allows to refine the view on a single molecule on-the-fly (i.e. change the representation of a molecule from a spherical shape to a more refined multi-center shape; an example could be the simulation of water as single sphere or as 3-center molecule to represent hydrogen and oxygen more accurately). This coupling will extend the range of applicability of MaMiCo considerably.
Objectives:

- Getting familiar with MD and the basic idea of molecular-continuum simulations
- Getting familiar with the software MaMiCo and with ESPResSo++ (both are C++-based)
- Implementing interfaces to couple MaMiCo and ESPResSo++ and setting up tests to verify and validate the coupling
- Running transient coupled simulations with the new coupling; a corresponding coupling has already been set up and can be re-used/adapted
- Running a transient coupled simulation with the new coupling and with ESPResSo++ making use of the adaptive resolution scheme

Further reading:

- P. Neumann et al. MaMiCo: Software design for parallel molecular-continuum flow simulations. Computer Physics Communications 200, pp. 324-335, 2016
- P. Neumann, X. Bian. MaMiCo: Transient Multi-Instance Molecular-Continuum Flow Simulation on Supercomputers. Computer Physics Communications 220, pp. 390-402, 2017
- C. Junghans, S. Poblete. A reference implementation of the adaptive resolution scheme in ESPResSo. Computer Physics Communications 181, pp. 1449-1454, 2010
- Software: www.espresso-pp.de, https://data.mendeley.com/datasets/w7rgdrhb85/1

Start time: anytime
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