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Student/Master Project: Implicit Time Coupling Scheme for Hybrid Molecular-continuum Simulations

Description: Compared to stand-alone continuum-based flow simulations, a lower level of spatial and temporal scales can be reached through a hybrid coupling of molecular dynamics (MD) and computational fluid dynamics (CFD). On the computational side, these coupled simulations bring many challenges in terms of parallelization, communication, memory access and/or storage efficiency. For example, the MD simulation requires to be executed over hundred thousands of time steps, while CFD simulations exhibit only 1-2% of the respective time steps; however, CFD simulations typically require to be computed on a large domain.
MaMiCo [1] is an open-source C++ framework for coupling MD and continuum solvers which allows, among others, good encapsulation of the coupling methods and massively parallel computations. Since recent developments, the multi-physics coupling library preCICE [2] has been coupled to MaMiCo. CFD solvers that are coupled with preCICE can now be coupled with MD solvers that are coupled with MaMiCo.
Among other new functionalities, preCICE supports implicit time coupling schemes. I.e., single time intervals are repeatedly simulated so that convergence between MD and CFD solver are guaranteed over the respective time interval. In this project the implicit coupling shall be explored, e.g. in terms of stability properties, time interval restrictions and fluctuations on MD side.

Prerequisites: basics of numerical mathematics; C++ programming skills; Linux/shell skills

Contact: Chair for High Performance Computing
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References:

[1] P. Neumann, X. Bian, MaMiCo: Transient multi-instance molecular-continuum flow simulation on supercomputers. Computer Physics Communications 220, pp. 390-402, 2017
[2] H-J. Bungartz, B. Gatzhammer, F. Lindner, M. Mehl, K. Scheufele, A. Shukaev, B. Uekermann. preCICE - A Fully Parallel Library for Multi-Physics Surface Coupling. Computers & Fluids 141, pp. 250-258, 2016