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Student/Master Project:
FabMaMiCo: Workflow Automation for Molecular-continuum Flow Simulations

Description:

FabSim3 [1] is an automation tool that reduces manual steps required for many tasks in computational science, such as pre- and postprocessing of data and running numerical simulations on remote machines. This helps to reduce the risk of human errors, to simplify workflows and to make research results more reproducible. The Python plugin system of FabSim3 allows to support additional applications via an API.

MaMiCo [2] is a C++ coupling framework designed to enable massively parallel flow simulations on HPC clusters, where a small molecular dynamics simulation is embedded in a larger computational fluid dynamics domain.

The goal of this project is to develop the new FabSim3 plugin 'FabMaMiCo', which allows to automate the processes of installing and compiling MaMiCo on remote machines, running MaMiCo based simulation jobs, managing a large ensemble of simulation configurations, retrieving and analyzing simulation results.

Prerequisites: At least rudimentary C++ programming skills, good Python and Linux shell skills required. Experiences with HPC clusters or numerical simulations are helpful, but not strictly required.

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References:

[1] D. Groen et. al. FabSim3: An automation toolkit for verified simulations using high performance computing. Computer Physics Communications 283, 2023. https://www.sciencedirect.com/science/article/pii/S0010465522003150

[2] P. Jarmatz et al. MaMiCo 2.0: An enhanced open-source framework for high-performance molecular-continuum flow simulation. SoftwareX 20, 2022. https://www.sciencedirect.com/science/article/pii/S2352711022001698