Student/Master Project:
Designing a scenario editor for the coupling tool MaMiCo

Description: The macro-micro coupling tool MaMiCo [JAR22] is software used to simulate physical systems where full molecular simulations are deemed expensive or unnecessary. MaMiCo runs coupled simulations between two solvers on the same physical domain: MD (molecular dynamics) solvers on volumes requiring higher scrutiny, and CFD (computational fluid dynamics) solvers on the remaining domain.

The coupling architecture is sound, however MaMiCo will benefit greatly from a robust scenario designing framework, to simplify designing simulations and specifying initial conditions. This will greatly increase accessibility, since currently only researchers well versed in MaMiCo can design novel simulations.

Students will be required to scrutinize the existing scenarios implemented within MaMiCo, and using them as a guideline to develop a framework for arbitrary scenarios with a variety of initial conditions. The emphasis is on code modularity, accessibility and sustainability.

Prerequisites: Modern C++ programming skills, experience in handling bigger software frameworks

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References:
[JAR22]   P. Jarmatz, H. Wittenberg, V. Jafari, A. D. Sharma, F. Maurer, N. Wittmer, P. Neumann. MaMiCo 2.0: An enhanced open-source framework for high-performance molecular-continuum flow simulation. SoftwareX 20, 101251, 2022