

MaMiCo-preCICE coupling for hybrid molecular-continuum flow simulations

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Compared to stand-alone continuum simulations, a lower level of spatial and temporal scales can be reached through a hybrid coupling of molecular dynamics and continuum fluid simulations. Such local molecular refinement simulations have diverse applications : engineering, polymer physics, complex molecular fluid modeling, micro-and nano-fluid networks or nanofiltration. A typical approach for such simulations is the coupling between a Computational Fluid Dynamics (CFD) software and a Molecular Dynamics (MD) software, which is challenging in many ways. Applications come with different requirements in the underlying CFD and MD solvers such as coupling algorithms, 2D vs. 3D, steady state vs transient simulations, etc. On the computational side, they bring many challenges in terms of parallelization, communication, memory access and/or storage efficiency. For example, the MD simulation requires to be executed for hundred thousands of time steps more than the CFD simulations or the CFD simulation needs to be computed on a large domain. MaMiCo [1] is an opensource C++ framework for coupling MD and continuum solvers which allows, among others, good encapsulation of the coupling methods and massively parallel computations.

In this work, we present the new preCICE [2] adapter for MaMiCo. It allows us to access the large number of continuum software already coupled to preCICE, to use preCICE features such as unstructured grids or interpolation methods or to have a real partitioned execution with separate executables inside MaMiCo. A Couette channel flow scenario allows us to test and validate our solution and shows good agreement with a reference solution.

REFERENCES

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¹<https://github.com/precice/precice/>

²<https://github.com/HSU-HPC/MaMiCo>