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Registration for PinT 2022

Dear Martin Gander and Florence Hubert,

thank you for announcing the PinT 22, 11th conference on Parallel-in-Time Integration.
I would love to join and propose a contributed talk:

Title

MaMiCo: Two-Way Coupled Parallel-in-Time Molecular-Continuum Flow Simulation

Abstract

In the area of multiscale computational fluid dynamics, coupled molecular-continuum flow simulations are an indispensable tool. They extend the applicability of pure molecular dynamics (MD) simulations to larger simulation domains and time scales, using a continuum flow solver. Due to their computational demand, massively parallel execution on high-performance computing systems is desirable, but spatial domain decomposition approaches offer a limited scalability.

In 2019, Blumers et al proposed the SPASD algorithm which is based on Parareal and enables parallel-in-time particle simulation using a continuum solver as a hydrodynamic predictor to supervise the microscopic system. Unlike traditional Parareal, SPASD uses additional mapping and projection operators as well as noise filtering to translate between the microscopic state and the macroscopic state. Thus, the two models can be inconsistent and solve different underlying governing equations.

In this talk, we present a concept that applies a modified SPASD variant to coupled molecular-continuum flow. Here, the macroscopic solver has two functions simultaneously: It is the coarse propagator in the predictor-corrector paradigm used for time parallelization, but it also extends the spatial domain of the simulation to scales beyond the limit of the particle system. We aim to implement our approach in the open-source C++ coupling framework MaMiCo, to demonstrate that it enables enhanced scalability for modular coupled 3D flow simulations, independent of the underlying continuum and particle codes.

I hope to see you next July in Marseille :)

Best regards
Piet Jarmatz