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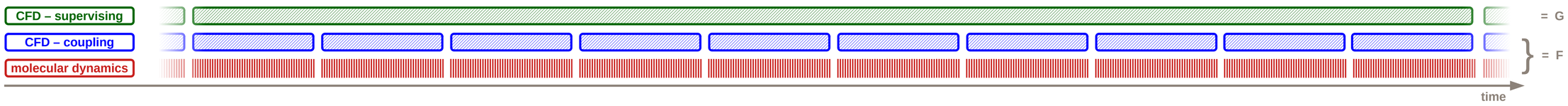
MaMiCo: A PinT Implementation for Molecular–Continuum Flow Simulation

Open source multiscale fluid simulation framework – Parallelized in five dimensions on supercomputers – Supervised parallel-in-time method with a variant of Parareal – Pushing computational limits of molecular dynamics in space and time

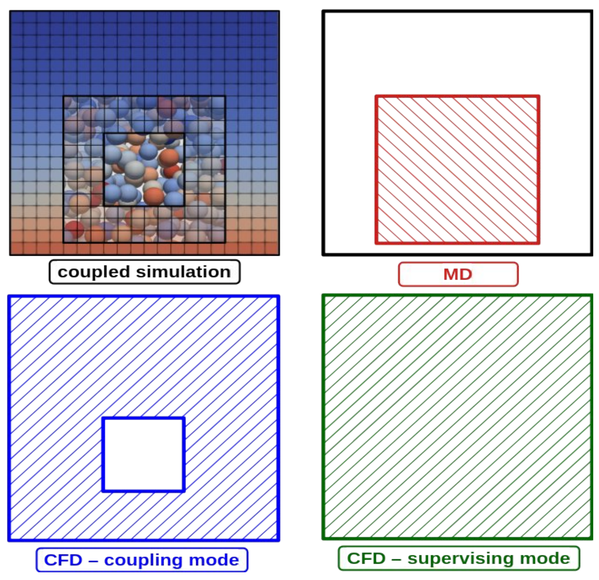


Idea and Concept

Coupling molecular (MD) and continuum flow simulation methods allows the investigation of atomistic effects in scenarios beyond computational limits of pure particle systems. Despite many other available options for parallelization (three spatial dimensions and independent MD simulation instances), the large number of required sequential time steps, in many cases, limits its scalability of molecular-continuum methods on supercomputers.

SPASD (Blumers et al., 2019) is a PinT algorithm for stochastic dynamics, where the particle system is supervised by a macroscopic model whose underlying governing equations are different from those of the microscopic model. SPASD differs from traditional Parareal by additional mapping, filtering and projection operators which essentially make the two models compatible.

Simulation Setup



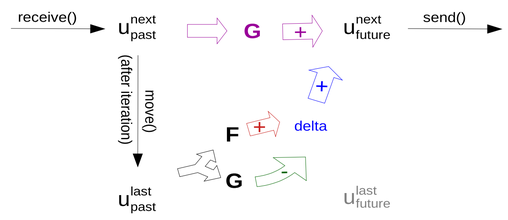
Our main idea is to apply SPASD in order to enable parallel-in-time two-way coupled molecular-continuum simulation. The macroscopic solver is used for both extending the MD domain in space, as well as supervising the coupling in time. The existing coupling methodologies, e.g. particle insertion (USHER), momentum relaxation, advanced noise filtering (POD, NLM) and special boundary conditions, are reused.

Methods

On the CFD side we use a Lattice Boltzmann (LB) method in a Couette flow test case here. We denote the state of the coupled LB simulation (i.e. a D3Q19 PDF field on 22x22x22 cells, 202 312 scalar values, including data from MD) as **u**, LB in supervising mode as **G** and the coupled simulation (MD + CFD) as **F**, then Parareal can be written as shown in Figure 1.

Implementation

We use the open source molecular-continuum coupling framework 'MaMiCo' to implement this PinT method in a generic way – independent of the underlying particle simulation code, CFD solver, and spatial parallelization. From the perspective of a single Parareal iteration on a single time domain:



This can be expressed in C++, for example:

```
while(!termination_criterion()){
    // Correction step
    auto delta = F(u_last_past) - G(u_last_past);

    // Prediction step
    receive(u_next_past);
    auto prediction = G(u_next_past);

    // Refinement step
    u_next_future = prediction + delta;
    send(u_next_future);

    // move for next iteration
    u_last_past   = std::move(u_next_past);
}
```

Due to the hydrodynamic statistical noise stemming from the particle system, the iteration termination criterion must take into account a tolerance such as

$$\frac{\|G(u_n^{k+1}) - G(u_n^k)\|}{\|G(u_n^{k+1})\|} < C_{tol}$$

For our example test case we use the constant flow channel height H=50, wall velocity u_w=1.5, fluid viscosity v=2.63, and coupling cycle time length dt=0.25. We can derive the analytical solution from the Navier–Stokes equations.

$$\bar{u}(t) = \frac{u_W}{2} - \frac{2u_W}{\pi}\sum_{k=1}^{\infty}\frac{1-\cos(\pi k)}{\pi k^2}\mathrm{e}^{-k^2\pi^2 \nu dt\, t/H^2}$$

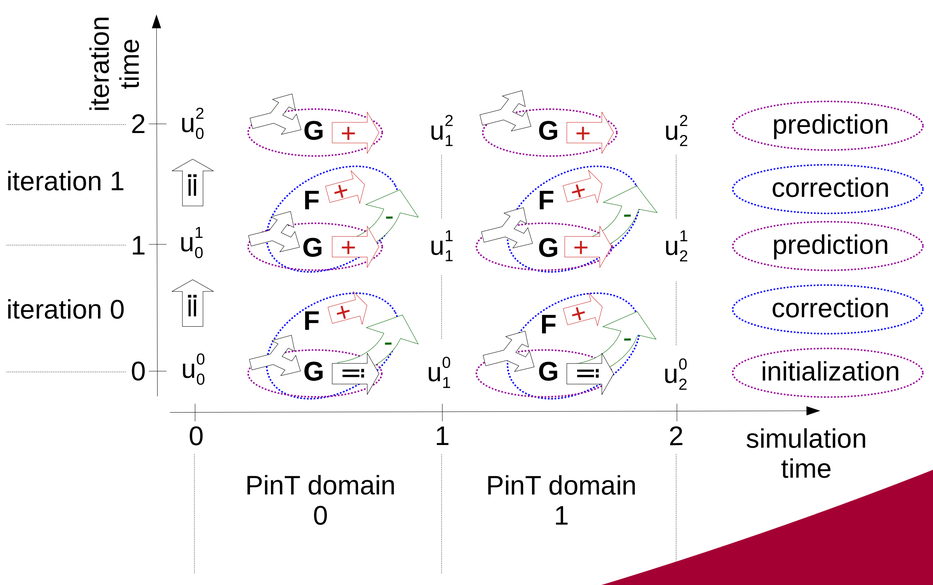
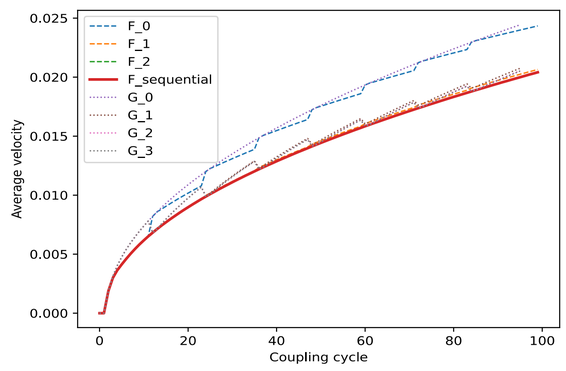


Figure 1: Parareal

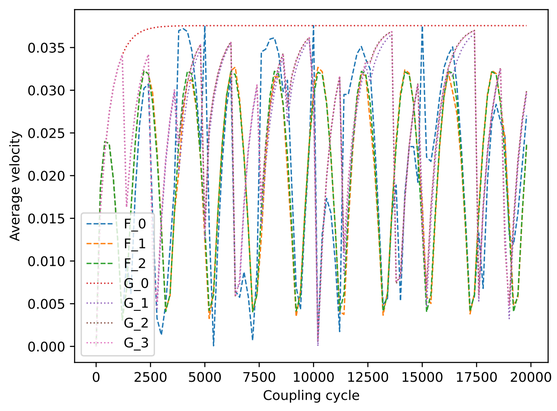
Results

We split the simulation time into 8 separate PinT domains and set the viscosity of G to 50% higher than F. The modified viscosity helps to investigate the effect of model differences between the two solvers. We plot the average flow velocity of all cells of the 3D simulation domain (vector magnitude).



We can use the analytical solution to validate the accuracy of this (one-way) coupled simulation result data. After three Parareal iterations, the relative error is 0.122 %.

As a more challenging test scenario, we set up a Couette flow with an oscillating wall velocity for F, but keep the wall velocity of G constant. We can compute 10^6 MD timesteps for two MD simulation instances with 21952 particles each, in 48 minutes on a single node of our cluster *HSUper*. The results demonstrate that even with the severe model error in the supervisor G, after a few Parareal iterations the method converges towards the oscillating flow.



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MaMiCo @ Github
https://github.com/HSU-HPC/MaMiCo

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