All Good Things Come in Threes:

Technische Universiteit Eindhoven University of Technology

Current Software and Algorithmic Developments for Molecular Dynamics–Lattice Boltzmann Simulations

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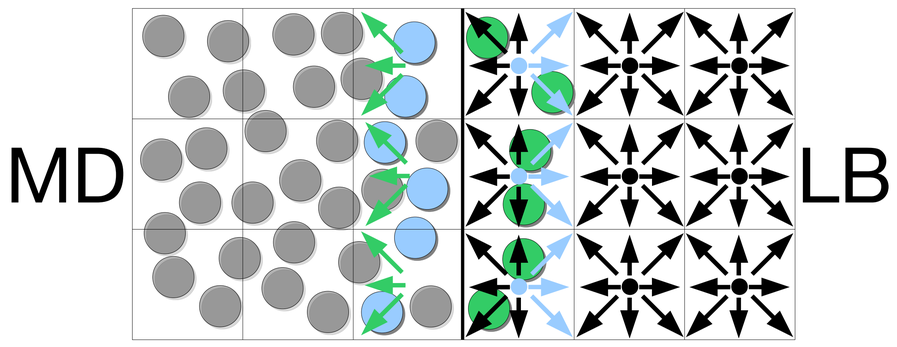
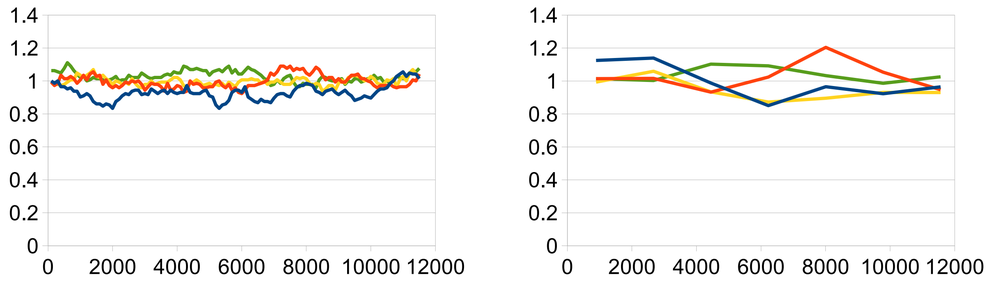
Overview

We present three branches of current research in the field of hybrid molecular dynamics–Lattice Boltzmann (MD–LB) simulations.
The first branch deals with the coupling of two in-house solvers – an adaptive Lattice Boltzmann (LB) implementation within the Peano framework [2] and a molecular dynamics (MD) solver MarDyn [1] – based on the hybrid scheme presented in [4]. With the MD solver allowing for massively parallel simulations [1], this project is considered to be a starting point for large scale hybrid molecular–continuum simulations.
The second branch is dedicated to a new flux-based coupling strategy for MD–LB systems [7]. In contrast to most coupling methods, we abstain from using MD overlap regions to increase computational and memory efficiency.
Modified Zou-He conditions [8, 6] are used to reconstruct missing particle distributions on the LB side from the transferred molecular quantities and known LB populations.
On the MD side, mass coming from the LB simulation is inserted via the USHER algorithm [3] and the transferred momentum is directly applied to the molecules near the boundary region. We use the method described in [5] to exert the correct hydrodynamic pressure near the sharp MD–LB interface. The poster describes the new coupling strategy and presents first results.
The third branch describes MaMiCo, a tool under current development which is written in C++ and is meant to allow for distributed parallel **Ma**cro-**Mi**cro-**Co**upling of different continuum and molecular dynamics solvers. It supports 2D and 3D setups and includes controller and insertion mechanisms for mass and momentum transfers between macroscopic and MD solvers. We present the basic concept and layout of MaMiCo.

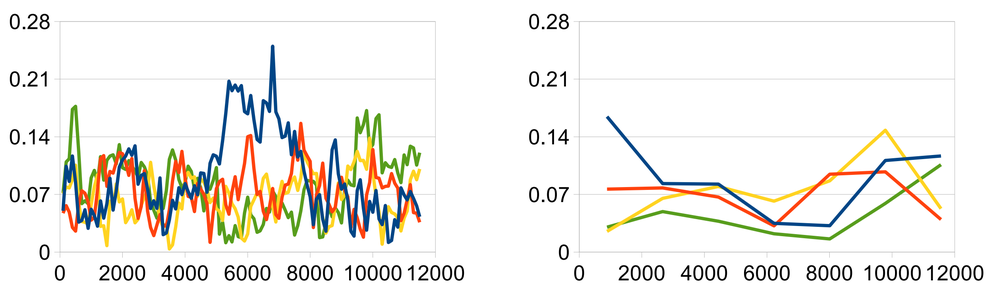
Molecular Dynamics–Lattice Boltzmann Simulations: A Flux-Based Approach



- On MD side:
  - Use (green) distribution functions from LB to compute mass and momentum flux
  - Insert mass (see [3], blue molecules) and momentum into MD region near MD–LB interface
  - Set hydrodynamic pressure force near MD–LB interface according to [5]
- On LB side:
  - Collect (green) molecules from MD simulation in buffer of LB cells and delete them from MD simulation
  - Use Zou-He conditions to reconstruct missing (blue) distribution functions from mass and momentum given by black distributions and MD buffer
  - To conserve mass, also the rest population (blue circle) needs to be reconstructed

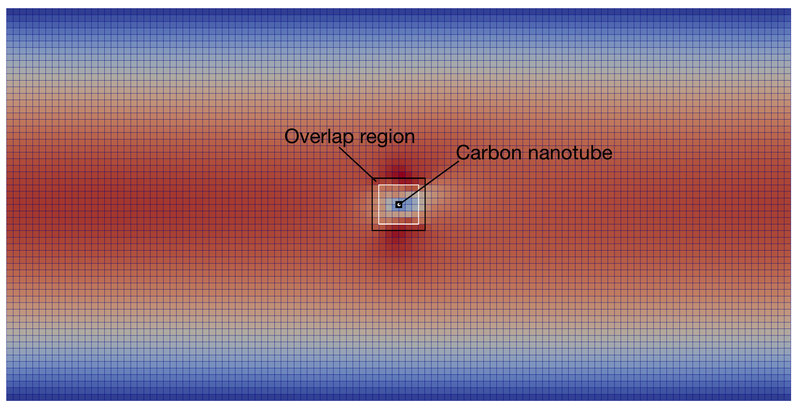


Density in MD (left) and LB (right) domain, measured over time in four near-interface cells for a fluid-at-rest scenario [7].



Velocity magnitude in MD (left) and LB (right) domain, measured over time in four near-interface cells for a fluid-at-rest scenario [7].

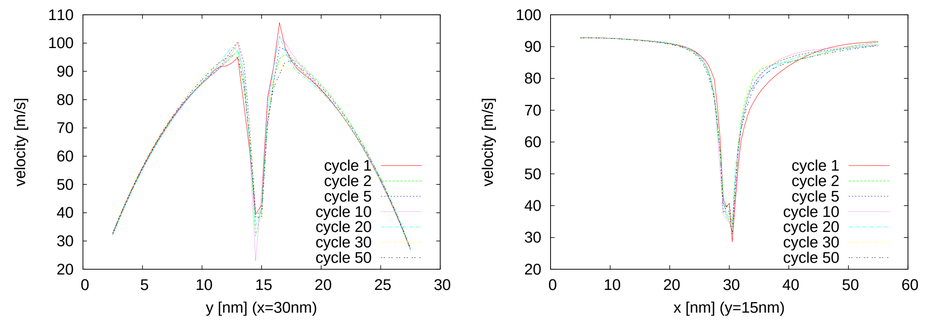
Hybrid Molecular–Continuum Simulations With Peano and MarDyn



Channel flow past a carbon nanotube. The region near the tube is resolved by MD (7957 molecules) whereas the outer region is solved by LB.

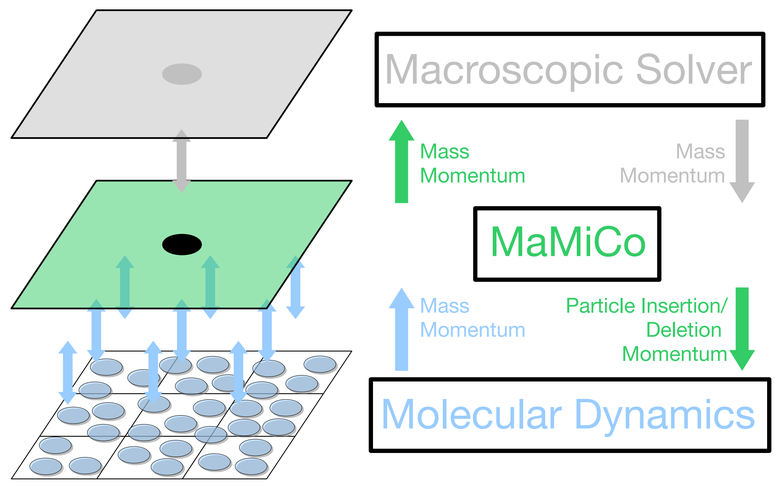
Coupled MD–LB simulations based on an iterative Schwarz domain decomposition [4]:

- LB implementation within Peano framework [2]
  → adaptive formulation, 2D/ 3D setups, different collision models (BGK,MRT)
- MD implementation MarDyn [1]
  → flexible molecular model and potential descriptions, massively parallel simulations, various applications in chemical engineering

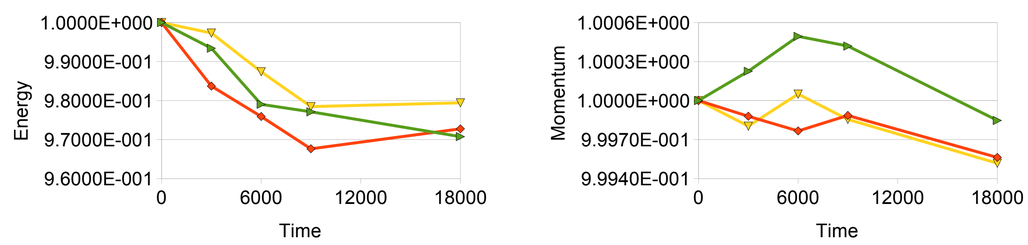


Evolution of the hybrid velocity profile in the planes located at x = 30nm (left) and at y = 15nm (right) over several Schwartz cycles.

MaMiCo: Macro-Micro-Coupling Tool



- C++-development for spatiotemporal hybrid molecular–continuum simulations
- Support of 2D/ 3D hybrid scenarios
- Macroscopic cells within MaMiCo are used to
  - map macroscopic quantities between the macroscopic solver and MaMiCo
  - map macro-/microscopic quantities between the MD solver and MaMiCo
- Particle insertion/ deletion [3] encapsulated within MaMiCo
- Coming soon: Distributed memory parallelisation



Normalised kinetic energy and momentum over time in particle insertion test (increase particle density $\rho(t = 0) = 0.35$ to $\rho(t = 9000) = 0.7$, equilibrate for another 9000 timesteps).

References

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