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Coupling lattice Boltzmann and atomistic models for fluids

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While dealing with fluid-structure interaction it was discovered that the macroscopic continuous boundary conditions at the interface fail at the microscopic scale [1]. A possible solution is the description of the interaction on atomistic level. Unfortunately, this approach is computationally expensive and only allows one to simulate small sub-domains while for the whole domain a coarse description is necessary. In this contribution, an approach for coupling the mesoscopic lattice Boltzmann method (LB) with the atomistic description for fluids (MD) is presented. The domain is split into two partially overlapping sub-domains. The overlapping is used to exchange the information between solutions which leads to the coupling between the models.

One of the strategies applied to match solutions in coupled simulations is Schwarz alternating method [5], where the values from the one domain are used as boundary condition for the other. In the present approach, a weak coupling is applied which translates fields between sub-domains by means of L2-projection [6]. A continuous field is built in the overlapping using linear shape functions and based on the unstructured mesh of particle positions of atomistic solution. The field is then mapped to the structured mesh of mesoscopic model where the values are eventually used as coupling control parameters for LB model. Thus, an iterative procedure of the alternating method is avoided. Moreover, the weak coupling method shows more stability than point-wise coupling of different length-scales [6].

For a mesoscopic sub-domain the isothermal lattice Boltzmann method is used [2]. The collision term is described with BGK-approximation. In the overlapping sub-domain the coupling is enforced through matching the mass density and the linear momentum. The momentum is coupled by adding a force term to the discrete LB equation [3]. To couple the mass density, an extra term is added to the LB equation, which corresponds to the hydrodynamic Euler equation with mass generation.

The interaction at the atomistic scale is described by Lennard-Jones potentials. In the overlapping sub-domain extra viscous forces are introduced to couple the linear momentum. The mass balance between the MD model and LB model is achieved by removing and insertion of particles [4].

To test the presented approach an alternating LB/MD/LB-description of a plane flow field is analysed. Matching mass and velocity quantities on inflow and outflow demonstrate the successful transition of variables between coupled sub-domains.

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