

A hybrid simulation approach: coupling lattice Boltzmann and molecular dynamics

M. Hecht

Institute for Computational Physics, University of Stuttgart
Pfaffenwaldring 27, 70569 Stuttgart, Germany

Internal seminar, summer semester 2009

In microfluidics, i.e. when studying flow through setups on the micrometer scale and below, the flow often strongly depends on the details of the interactions between fluid and the confining walls. To incorporate these molecular details into a lattice Boltzmann (LB) simulation, we develop a hybrid simulation technique: We apply molecular dynamics (MD) in those regions, where the interactions are important and combine this with an LB simulation for the bulk to take advantage of the computational speed of the mesoscopic method.