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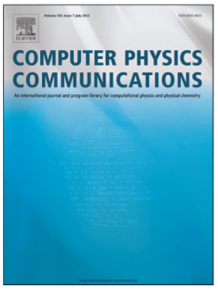

Molecular dynamics simulations in hybrid particle-continuum schemes: Pitfalls and caveats

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Molecular dynamics simulations in hybrid particle-continuum schemes: Pitfalls and caveats

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Abstract

Heterogeneous multiscale methods (HMM) combine molecular accuracy of particle-based simulations with the computational efficiency of continuum descriptions to model flow in soft matter liquids. In these schemes, molecular simulations typically pose a computational bottleneck, which we investigate in detail in this study. We find that it is preferable to simulate many small systems as opposed to a few large systems, and that a choice of a simple isokinetic thermostat is typically sufficient while thermostats such as Lowe-Andersen allow for simulations at elevated viscosity. We discuss suitable choices for time steps and finite-size effects which arise in the limit of very small simulation boxes. We also argue that if colloidal systems are considered as opposed to atomistic systems, the gap between microscopic and macroscopic simulations regarding time and length scales is significantly smaller. We propose a novel reduced-order technique for the coupling to the macroscopic solver, which allows us to approximate a non-linear stress-strain relation efficiently and thus further reduce computational effort of microscopic simulations.

Key words: shear flow, heterogeneous multiscale methods, Molecular Dynamics, discontinuous Galerkin method, soft matters

1. Introduction

Modeling and computational simulation of soft matter liquids remains a challenging problem because these fluids may exhibit complex non-Newtonian effects, such as shear-thinning/thickening, viscoelasticity or flow-induced phase transition. Such complex behavior is attributed to microstructure changes in fluids when a system is subject to an external mechanical shear force [28, 29]. Therefore, computational modeling of soft-matter fluids has to necessarily take into account microscopic effects in order to obtain reliable numerical solutions.

Clearly, the most accurate description of soft-matter fluids can be obtained by the molecular dynamics (MD). However, such microscale description is computationally inefficient, if large scale regions in space and time need to be simulated. To overcome this restriction and to obtain practically tractable simulation techniques hybrid molecular-continuum methods have been proposed in the literature aiming in combining the best attributes of both parts: the molecular accuracy with the computational efficiency of continuum models.

Bridging the large range of dynamically coupled scales is a fundamental challenge that is a driving force in the development of new mathematical algorithms. In general, hybrid models can be divided in two groups: based on the Eulerian-Lagrangian decomposition or on domain decomposition. In the first type the Lagrangian-type particles are embedded in the Eulerian fluid description, see, e.g., [14, 34, 42]. The second type of the methods is based on the domain decomposition into a small accurate atomistic region embedded into a coarser macrosopic model, see, e.g., [15]. In the literature we can find several hybrid models combining particle dynamics with the macroscopic continuum model, see, e.g., the hybrid heterogeneous multiscale methods described in [8, 6, 9, 11, 33, 34, 42], the triple-decker atomistic-mesoscopic-continuum method [15], the seamless multiscale methods [7, 10], the equation-free multiscale methods [22, 23] or the internal-flow multiscale method [2, 3]. In [24] a overview of multiscale flow simulations using particles is presented. The essential question that arises in building a coupled multiscale method is how micro- and macroscopic models are linked together, i.e., how projection/lift (or compression/reconstruction) operators are defined and implemented.

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