A Continuum-Atomistic Multi-Timescale Algorithm for Micro/Nano Flows[†]

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Abstract. A multi-timescale algorithm is proposed for simulating time-dependent problems in micro- and nano- fluidics. The total simulation domain is spatially decomposed into two regions. Molecular dynamics is employed in the crucial interfacial regions and continuum hydrodynamics is adopted in the remaining bulk regions. The coupling is through "constrained dynamics" in an overlap region. Our time scheme is based on the time scale separation between the continuum macro time step and molecular micro time step. This allows the molecular dynamics during one macro time step to be treated as in quasi-steady state. Therefore, molecular simulation is only performed in two shorter time intervals. Through linear extrapolation of macroscopic velocities and re-initialization of particle configurations, we can significantly reduce the total computational cost. We demonstrate and discuss our time algorithm through hybrid simulation of channel flow driven by a sinusoidally moving top wall. Converging results are achieved for cases of large separation of time scale with much less computational cost than with the original hybrid simulation without time extrapolation.

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1 Introduction

Continuum hydrodynamics with simple constitutive relations and no-slip boundary conditions is quite successful in describing macroscopic fluid flows, but may fail in many situations in micro and nano engineering where molecular detail is important. In principle, classical molecular dynamics (MD) can provide all the detailed information and is capable of resolving all the problems. However, performing a MD simulation on the required spatial and temporal scales is computationally impractical due to the extremely tiny spatial and temporal scales associated with molecular motion. It has been observed that in many common scenarios, molecular details are required only in small spatial regions such as solid-fluid or fluid-fluid interfaces, while the continuum descriptions are still accurate in the remaining bulk regions. Therefore, it is desirable to develop a hybrid method to combine the efficiency of continuum hydrodynamics and accuracy of MD simulation.

Several hybrid schemes have been developed for simulating dense liquid systems in the last decade. Most are based on "domain decomposition", in which the simulation domain is decomposed into two regions. MD is adopted in small crucial regions where molecular details are important and continuum hydrodynamics is used in the remaining bulk regions. A coupling algorithm must be developed to ensure the consistency of these two completely different descriptions, and this is the heart of all hybrid methods.

O'Connell and Thompson [1] suggested coupling via a finite overlap region to avoid sharp transitions and used a relaxation method to ensure consistency of velocities between MD and continuum regions. They successfully implemented their approach in simulating simple one dimensional Couette flow. Hadjiconstantinou and Patera [2] introduced a Maxwell Demon method and they employed a momentum reservoir to constrain the particle velocities. The Schwarz iteration method was adopted to ensure MD and continuum descriptions were consistent. Examples of steady state channel flow with obstacles [2] and moving contact-line problems [3] were used to demonstrated their method. Flekkoy *et al.* [4] proposed a coupling scheme based on the continuity of mass and momentum fluxes for simulating compressible flows. In their recent works [5,6], they also accounted for the energy flux in their examples. Buscalioni and Coveney [7,8] also adopted the flux coupling scheme and demonstrated their approach by simulation of transversal and longitudinal waves.

More recently, Nie *et al.* [9] developed a coupling scheme using Lagrange multipliers for simulating isothermal, incompressible flows. In their approach, the particle velocities were constrained in the overlap region such that the average particle velocities were equivalent to the instantaneous continuum velocities. They have successfully implemented their approach for simulating driven cavity flow [10,11] and moving contact-line problems. Most recently Liu *et al.* [12] extended the scheme developed in [9] to incorporate thermal effects. Based on Nie *et al.* 's work [9], several minor modifications of the constrained equations have also been proposed. Wang and He [13] proposed a dynamic coupling model in which the coupling parameter in the constrained equations