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Fluid simulations with atomistic resolution: a hybrid multiscale method with field-wise coupling ☆

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ABSTRACT

We present a new hybrid method for simulating dense fluid systems that exhibit multiscale behaviour, in particular, systems in which a Navier–Stokes model may not be valid in parts of the computational domain. We apply molecular dynamics as a local microscopic refinement for correcting the Navier–Stokes constitutive approximation in the bulk of the domain, as well as providing a direct measurement of velocity slip at bounding surfaces. Our hybrid approach differs from existing techniques, such as the heterogeneous multiscale method (HMM), in some fundamental respects. In our method, the individual molecular solvers, which provide information to the macro model, are not coupled with the continuum grid at nodes (i.e. point-wise coupling), instead coupling occurs over distributed heterogeneous fields (here referred to as field-wise coupling). This affords two major advantages. Whereas point-wise coupled HMM is limited to regions of flow that are highly scale-separated in all spatial directions (i.e. where the state of non-equilibrium in the fluid can be adequately described by a single strain tensor and temperature gradient vector), our field-wise coupled HMM has no such limitations and so can be applied to flows with arbitrarily-varying degrees of scale separation (e.g. flow from a large reservoir into a nano-channel). The second major advantage is that the position of molecular elements does not need to be collocated with nodes of the continuum grid, which means that the resolution of the microscopic correction can be adjusted independently of the resolution of the continuum model. This in turn means the computational cost and accuracy of the molecular correction can be independently controlled and optimised. The macroscopic constraints on the individual molecular solvers are artificial body-force distributions, used in conjunction with standard periodicity. We test our hybrid method on the Poiseuille flow problem for both Newtonian (Lennard-Jones) and non-Newtonian (FENE) fluids. The multiscale results are validated with expensive full-scale molecular dynamics simulations of the same case. Very close agreement is obtained for all cases, with as few as two micro elements required to accurately capture both the Newtonian and non-Newtonian flowfields. Our multiscale method converges very quickly (within 3–4 iterations) and is an order of magnitude more computationally efficient than the full-scale simulation.

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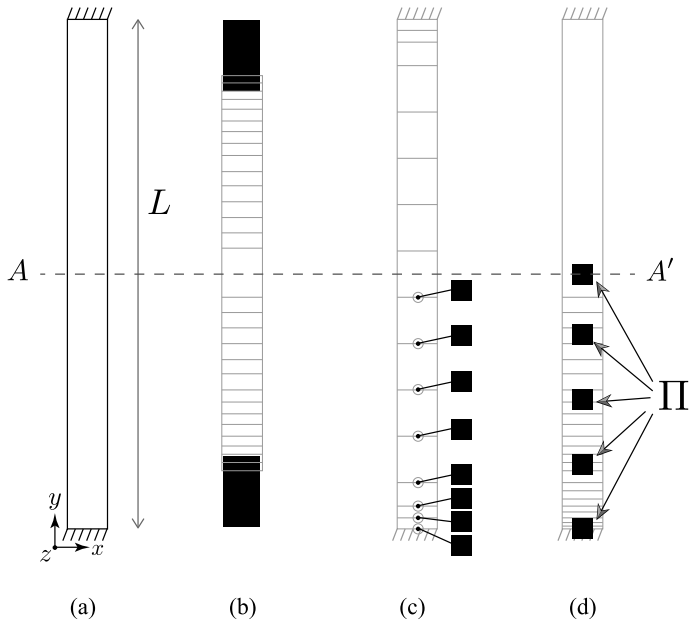

Fig. 1. Schematic of hybrid and multiscale methods in the literature, and our new multiscale approach proposed in this paper: (a) 1D Poiseuille flow problem; (b) Domain-Decomposition (DD); (c) Heterogeneous Multiscale Method (HMM) with point-wise collocated coupling; and (d) HMM with our Field-wise Non-collocated Coupling (HMM-FWC). The grey mesh indicates the macro domain, while black filled boxes indicate micro subdomains. A–A' is the line of symmetry.

1. Introduction

In an important class of fluid dynamics problems the overall physics is multiscale, in that microscopic processes strongly dictate the macroscopic behaviour. For example, granular flows in avalanches, shockwaves in high-speed rarefied flows, rain filtration through soil, etc. The present paper specifically focuses on micro- and nano-scale fluid dynamics, where atomistic processes occurring over pico- or nano-scales determine the bulk effects occurring over micro- and milli-scales, both temporally and spatially. The development of future technologies depending on nano- and micro-fluidics requires methods that resolve the multiscale phenomena accurately and efficiently.

Molecular Dynamics (MD) is now a recognised computational tool for accurately modelling fluid behaviour at atomistic scales as an ensemble of discrete molecules that obey fundamental laws of physics. In essence, a flow problem could be entirely described by such a microscopic model. While this is suitable for simulating small systems over short time-scales, such as water flows through carbon-nanotubes, in nano and micro engineering applications it becomes computationally intractable to resolve all the important space and time-scales involved.

In such flow problems, the continuum conservation laws can be used as an accurate, though incomplete, model for the macroscopic flow behaviour. Molecular dynamics can then be employed to replace, or close, equations in parts of the computational domain where a classical macroscopic constitutive or boundary model does not exist (e.g. liquids next to surfaces, rheological fluids, chemical reactions, etc). This is the so-called *hybrid methodology*, in which "the best of both worlds" in terms of computational cost and accuracy can be achieved by unifying disparate macroscopic and microscopic solvers in a coupled simulation.

The most common current approach to hybrid methods for dense fluids is domain-decomposition (DD) [1–6]. As the name implies, the computational domain is divided uniquely into macro and micro parts, providing only an overlapping region for matching hydrodynamic flux or state properties that act as Dirichlet or Neumann-type boundary conditions at the hybrid interface. Figs. 1(a) and (b) illustrate the DD method applied to a simple Poiseuille flow problem. Despite providing a reasonable rationale for modelling near-wall flows, DD schemes have some disadvantages. First, DD can only be used for flows that have a *bulk* flow region for which a constitutive model is known and is accurate. Furthermore, while it may be reasonably straightforward to segment a domain explicitly into micro/macro subdomains if it is a simple 1D system, it may be more challenging if the hybrid interface has more complex features [7]. Another issue is that of applying acceptable 'open-system' or 'macro–micro' boundary conditions at the non-periodic MD interface, which is a topic that is not well developed in the literature. Finally, DD methods do not generally work well for systems that exhibit varying degrees of scale separation, and can be of comparable computational cost to a full MD simulation of the case [8,9].

A different hybrid methodology that exploits the scale separation between molecular and continuum processes was proposed by E and co-workers [10,11]. This was dubbed the Heterogeneous Multiscale Method (HMM), and is illustrated in Fig. 1(c). The central idea of HMM is that continuum governing equations for mass, momentum and energy conservation are able to predict the overall macroscopic behaviour, with only the missing/unknown fluid-constitutive and boundary