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RESEARCH PAPER

An artificial neural network-based multiscale method for hybrid atomistic-continuum simulations

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Abstract This paper presents an artificial neural network-based multiscale method for coupling continuum and molecular simulations. Molecular dynamics modelling is employed as a local "high resolution" refinement of computational data required by the continuum computational fluid dynamics solver. The coupling between atomistic and continuum simulations is obtained by an artificial neural network (ANN) methodology. The ANN aims to optimise the transfer of information through minimisation of (1) the computational cost by avoiding repetitive atomistic simulations of nearly identical states, and (2) the fluctuation strength of the atomistic outputs that are fed back to the continuum solver. Results are presented for prototype flows such as the isothermal Couette flow with slip boundary conditions and the slip Couette flow with heat transfer.

Keywords Multiscale modelling · Hybrid methods · Molecular dynamics · Continuum fluid dynamics · Artificial neural networks

1 Introduction

Over the past decade, the study of micro and nanoscale flows has attracted significant scientific and industrial interest due to the increasing number of devices operating on small scales. Applications of micro and nanofluidic devices, for example, have benefited various disciplines spanning from nanomedicine to nanomanufacturing and environmental sciences (Kamholz et al. 1999; McClain and Sims and Ramsey 2003). Due to their large surface-to-volume ratio, the flows in these devices are sensitive to the surface properties. Improving our physical understanding of micro and nanoscale phenomena is thus essential for further exploiting the application of micro and nanofluidics (Nicholls et al. 2012; Gad-El-Hak 2006; Singh et al. 2008, Prasianakis and Ansumali 2011).

In the framework of continuum modelling the microscopic mechanics tends to be neglected and the microscopic effects are usually represented through averaged quantities such as viscosity and thermal conductivity (Sofos et al. 2009; Liu et al. 2007; Priezjev 2007). Therefore, as the operational dimensions are downsized to smaller scales, where the surface properties dominate the flow characteristics, the macroscopic constitutive relations and boundary conditions become inadequate and microscopic models, such as molecular dynamics (MD), have to be employed. Various MD studies have been presented in the literature with respect to effects of surface properties, such as wettability and nanoscale roughness and the slip generated in solid-fluid interfaces (Thompson and Troian 1997; Asproulis and Drikakis 2010; Priezjev et al. 2005; Yang 2006; Asproulis and Drikakis 2010; Niavarani and Priezjev 2010; Asproulis and Drikakis 2011; Nagayama and Cheng 2004; Sofos et al. 2012). However, the applicability of atomistic models to larger temporal and spatial scales is restricted due to their high computational cost (Asproulis et al. 2012; Asproulis and Drikakis 2009; Lorenz et al. 2010; Valentini and Schwartzentruber 2009; Koishi et al. 2005; Plimpton 1995). Aiming to confront the efficiency and accuracy limitations of the molecular and continuum models, respectively, and provide a unified description across the various scales, hybrid continuum-molecular approaches have been developed (Liu et al.

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