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RESEARCH PAPER

A hybrid molecular-continuum simulation method for incompressible flows in micro/nanofluidic networks

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Abstract We present a hybrid molecular-continuum simulation method for modelling nano- and micro-flows in network-type systems. In these types of problem, a full molecular dynamics (MD) description of the macroscopic flow behaviour would be computationally intractable, or at least too expensive to be practical for engineering design purposes. Systems that exhibit multiscale traits, such as this, can instead be solved using a hybrid approach that distinguishes the problem into macroscopic and microscopic dynamics, modelled by their respective solvers. The technique presented in this study is an extension and addition to a hybrid method developed by Borg et al. (J Comput Phys 233:400–413, 2013) for high-aspect-ratio channel geometries, known as the internal-flow multiscale method (IMM). Computational savings are obtained by replacing long channels in the network, which are highly scale-separated, by much smaller, but representative, MD simulations, without a substantial loss of accuracy. On the other hand, junction components do not exhibit this length-scale separation, and so must be simulated in their entirety using MD. The current technique combines all network elements (junctions and channels) together in a coupled simulation using continuum conservation laws. For the case of steady, isothermal, incompressible, low-speed flows, we use the conservation of mass and momentum flux equations to derive a set of molecular-continuum constraints. An algorithm is presented here that computes at each iteration the new constraints on the pressure differences to be applied over individual MD micro-elements (channels and junctions), successively moving closer to macroscopic mass and momentum conservation. We show that hybrid simulations of some example network cases converge quickly, in only a few iterations, and compare very well to the corresponding full MD results, which are taken as the most accurate solutions. Major computational savings can be afforded by the IMM-type approximation in the channel components, but for steady-state solutions, even greater savings are possible. This is because the micro-elements are coupled to a steady-state continuum conservation expression, which greatly speeds up the relaxation of individual micro-components to steady conditions as compared to that of a full MD simulation. Unsteady problems with high temporal scale separation can also be simulated, but general transient problems are beyond the capabilities of the current technique.

Keywords Multiscale simulations · Hybrid methods · Molecular dynamics · Coupled solvers · Scale separation · Microfluidics · Nanofluidics

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1 Introduction

Molecular dynamics (MD) is a useful numerical tool for probing microscopic phenomena and non-equilibrium dynamics in merging nano- and microfluidic technologies. MD can capture macroscopic hydrodynamics, or even operate as an ab initio tool for continuum-based solutions in which it provides the microscopic constitutive or