Advances and Challenges in Computational Research of Micro and Nano Flows

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Abstract This paper presents a collective overview of recent studies regarding the computational modelling of micro- and nano-fluidic systems. The review provides an introduction to atomistic, mesoscale and hybrid methods for simulating micro and nano-flows, as well as discusses recent applications and results from the application of such methods.

Keywords: Microflows, Nano-flows, atomistic, continuum, molecular dynamics, multiscale, Computational Fluid Dynamics (CFD), Monte Carlo, dissipative particle dynamics, hybrid methods

1. Introduction

Modelling fluid dynamics has long been a task considered in the framework of the Euler and Navier-Stokes equations, whose success in computer simulations aiming at understanding the physics of fluid dynamics and heat transfer, as well as in assisting with the design and optimisation of macroscopic structures and devices has established it as the most effective method for studying fluid flow. This approach, however, is based on the assumption of a continuum fluid which is in equilibrium at any point or infinitesimal volume, a premise reasonable at larger scales. As the fluid is restricted spatially to nano-meter sized characteristic dimensions, phenomena at interfaces, which occupy a significant percentage of the overall system, influence the homogeneous structure of the liquid particles and introduce dynamics that cannot be captured by continuum mechanics (Koplik, Banavar and Willemsen 1989, Travis, Todd and Evans 1997, Wang, Liu and Chen 2008)

Atomic scale simulation techniques such as Molecular Dynamics (MD) and Monte Carlo (MC) methods have proven effective in delineating, from first principles, the physical apparatus, which governs the dynamics of such systems, assisting in the resolution of discrepancies between experimental results and macroscopic computational models. Examples include the study of the structure of the liquid particles close to the solid-liquid interface, which was found to be stratified parallel to the channel walls (Bitsanis, et al. 1987, Asproulis and Drikakis, Boundary slip dependency on surface stiffness 2010, Asproulis and Drikakis, Wall-mass effects on hydrodynamic boundary slip 2011, Sofos, Karakasidis and Liakopoulos 2009). This reconciled experimental observations (Doerr, et al. 1998, Henderson and van Swol 1984) and assisted in a better understanding of the properties of the system such as stiffness of the wall and the strength of interaction between the wall and liquid atoms. The slip of the liquid across the solid surface was also studied (Asproulis and Drikakis, Boundary slip dependency on surface stiffness 2010, Asproulis and Drikakis, Wall-mass effects on hydrodynamic boundary slip 2011) and, along with experimental data (Choi, Westin and Breuer 2003), has urged a reconsideration of the circumstances under which the no-slip condition, often employed in macroscopic simulations, renders a physically meaningful constraint. The thermodynamics of nanofluidic scenarios have also been found to deviate from the expectations of continuum models. Flow through nanochannels has indicated the existence of a heat flux, even in the absence of a temperature gradient across the two walls, due to variations in the temperature profile which result from viscous heating (Baranyai, Evans and Daivis 1992, Todd and Evans 1997). The thermal resistance across the solid-liquid interface has also been found to be strongly coupled with the wettability of the solid surface (Barrat and Chiaruttini 2003), the density of the liquid and the wall stiffness (Kim, Beskok and Cagin 2008). Furthermore, the thermal conductivity of confined liquids has been found to be dependent on the channel-width (Sofos, Karakasidis and Liakopoulos 2009), as well as to be highly

anisotropic with the thermal conductivity in the normal-to-the-wall direction being impaired as a result of the reduced diffusion coefficient due to confinement (Liu, et al. 2005).

The main disadvantage of atomic-scale simulation methods is their computational expense, which increases exponentially with the size of the simulation domain. Hence, complications arise in micro-flows in which the non-homogeneities and interfacial effects of nano-flows are still evident.

This blend of difficulties in such systems makes the independent use of either continuum or atomistic methods insufficient or practically impossible. To account for this, mesoscale and hybrid molecular-continuum methods (HMCM) have been of academic interest for over two decades now. These methods attempt to couple the two types of models, thus allowing for an accurate calculation of the properties of the system at reduced computational cost. Mesoscale models comprise a single solver, which attempts to give a more efficient solution based on atomistic observations, while HMCM utilises both molecular and continuum solvers exchanging information. FIG. 1 schematically shows the time and length scales in which atomistic, continuum and hybrid methods are used.

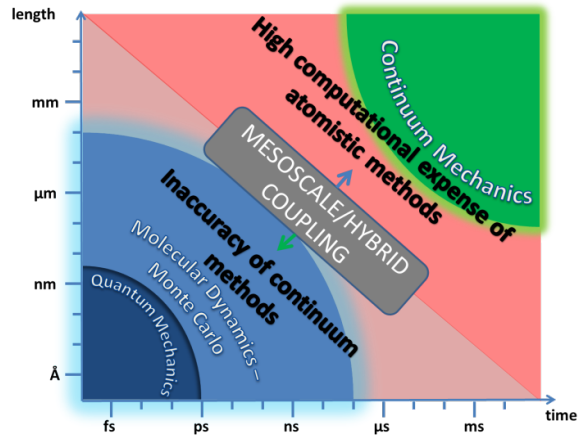

FIG. 1 Time and length scales of computational methods for micro and nano fluids.

This paper introduces atomistic, mesoscale and hybrid techniques, and gives an overview of the most recent findings and results of such methods for micro- and nano-fluidics.

2. State of the art methods for micro and nano flows

The computational methods for micro and nano flows are into three main categories: continuum; atomistic; and multiscale methods; the latter include mesoscale and HMCM models.
In the framework of continuum mechanics, CFD is used to describe the fluid motion. For the vast majority of cases, this is achieved through the solution of the Navier-Stokes equations. However, for more complex systems, such as rarefied gases, the Lattice-Boltzmann Methods (LBM) can be employed instead.

In systems where microscopic processes are important (i.e. solid-liquid interfaces in nanochannels), a more fundamental approach is required to capture the physical phenomena that give rise to macroscopic observations. In general, these methods treat each atom or molecule as a fundamental particle and the interactions between them are dictated by empirical potentials derived from fitting material properties from experimental observations or quantum mechanical calculations (ab initio).

A common atomistic approach is the stochastic Monte Carlo (MC) method (Allen and Tildesley 1989). Based on the initial positions of the particles and their pre-defined potentials, the total potential energy of the system is calculated. MC then randomly changes the position of a particle and accepts the new state if its potential energy is less than the previous. The repetition of this procedure is responsible for the evolution of the system.

In contrast to MC which is a stochastic model, Molecular Dynamics (MD) is a deterministic method in which the system evolves based on Newton's laws of motion (Allen and Tildesley 1989). It is the only method which attaches timescales to the various phenomena, hence it can determine the dynamical behaviour of the system, allowing for the estimation of properties such as the relaxation time of various system quantities (i.e. momentum, microscopic heat flux).

Both MC and MD are established techniques, with respect to the evolution of the system.The main challenges lie in the accurate representation of the model, achieved through a suitable choice of interatomic potentials, and through the correct application of statistical mechanics for the retrieval of meaningful quantities.

Although monatomic liquids such as Argon are often used to capture generic properties of flows under certain conditions, a large body of work is focused on the modelling of more complex fluids and solutions (Feng and Voth 2010). Complex nanofluids such as hexagonal boron nitrid (h-BN) suspended in mineral oil have been successfully modelled to be studied as possible cooling fluids in electrical transformers (Raji, et al. 2012).

In addition investigations have gone to great lengths to accurately model walls which interact thermally with the liquid and can control its temperature without the use of thermostats or any other artifacts applied to the liquid, physically portraying the thermodynamic behaviour of the system (Kim, Beskok and Cagin 2008).

Mesoscale schemes usually introduce the notion of pseudo-particles, which represent larger portions of the actual system, thus reducing the computational cost. Dissipative Particle Dynamics (DPD) is such a mesoscopic pseudo-particle method in which each particle in the system represents a cluster of atoms or molecules. Unlike MD, DPD is governed by three types of forces: the conservative, which dictates the interatomic interactions between the pseudo-particles and the dissipative and random forces which together act as a thermostat of the system (Hoogerbrugge and Koelman 1992).

DPD is becoming continuously more popular in the description and investigation of micro and nanoflows. Although the resolution of the method is much lower than that of MD models, simulations of complex molecular structures such as polymeric systems (Fellermann, et al. 2007) has also been performed. Adjustments of the boundary conditions also allow for a tunable slip velocity for fluids in nanochannels, portraying a more physically accurate system (Ranjith, Patnaik and Vedantam 2013).
In addition to mesoscale methods, HMCM have been developed which combine both, atomic (MD or MC) and continuum (CFD) solvers. The idea is to minimize the use of the computationally expensive MD, achieved by allocating it only small regions or time-frames to operate in.

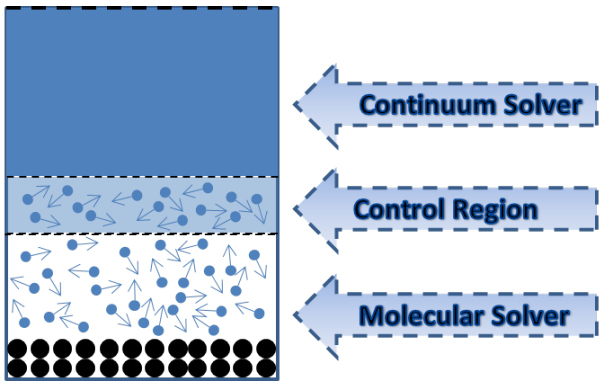

FIG. 2 Schematic representation of a geometric decomposition approach

HMCM methods are broadly divided into geometric decomposition (GD) or pointwise coupling (PWC). GD splits the domain into regions, the largest ones being allocated to the continuum solver leaving some parts of the simulation box for the molecular solver. An in-between region, called the control region, is used to enforce continuity between the molecular and continuum blocks. The information between the various regions is shared through a hybrid solution interface (HSI). FIG. 2 schematically shows the various regions of a GD model. The PWD method uses the continuum solver for the entire domain and the molecular solver is used at specific nodes or cells as a refinement.

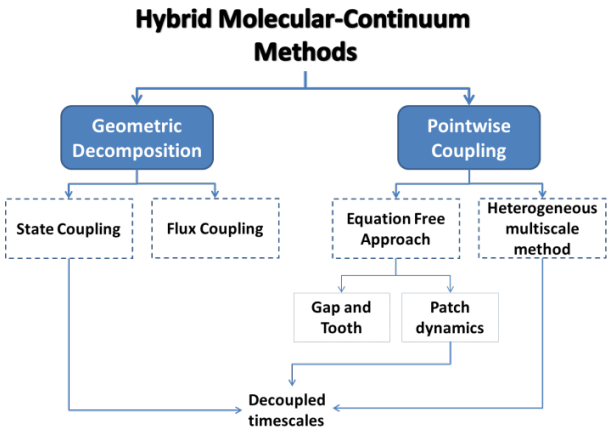

FIG. 3 A schematic representation of the general subdivisions of HMCM.

HMCM increasingly become more popular as they can simulate practical scenarios and aid in the design and manufacture of components. New models exist for describing micro and nano flows of high aspect ratio (Borg, Lockerby and Reese, A multiscale method for micro/nano flows of high aspect ratio 2013a), Kalweit & Drikakis, 2008-2011, Asproulis & Drikakis, 2011). HMCM achieves a significant reduction in computational resources by restricting the use of MD only to a limited number of streamwise-distributed cross-sections. The model was further extended to compute flows through networks of micro and nano channels, a daunting task to be carried out purely by MD (Borg, et al., 2013b, Kalweit & Drikakis, 2011). A hybrid model has also been presented for incompressible non-isothermal steady-state flows which does not require the calculation of the Irving-Kirkwood stress tensor or heat flux vector (Alexiadis, et al. 2013). The method, which is a PWC-based scheme, works by calculating the velocity and temperature Laplacians at internal nodes and the velocity and temperature values at boundaries. The model was validated by simulating flow in a channel with a temperature difference between the walls. A new hybrid MC-continuum approach has also been published (Darbandi and Roohi, A hybrid DSMC/Navier--Stokes frame to solve mixed rarefied/nonrarefied hypersonic flows over nano-plate and micro-cylinder 2013) capable of solving the mixed non-equilibrium and near-equilibrium flow regions efficiently.

3. Recent findings and results in micro and nano flows

The wide spectrum of applications of micro and nano-flows, ranging from biology and biotechnology (Mills, et al., 2013, Benke et al, 2008, 2013, Barton et al, 2011, Selimovich et al. 2011) to cooling devices (Tuckerman and Pease 1981) have sparked academic and industrial interest in the fluid flow through such devices.

The conditions for fluid slippage across a solid interface have been studied intensively over the past decade. With the aid of MD, a sensitivity analysis has been carried out indicating how system parameters such as the properties of the channel walls can influence the mobility of the fluid particles at the interface (Asproulis and Drikakis, Wall-mass effects on hydrodynamic boundary slip 2011, Sofos, Karakasidis and Liakopoulos 2009). It has recently been observed that the slip of oscillatory Couette flows is well described by the Stokes flow solution and the slip length is correlated with the local shear rate (Priezjev, Molecular dynamics simulations of oscillatory Couette flows with slip boundary conditions 2013). Such flows, however, assume perfectly flat walls. Non-Equilibrium Molecular Dynamics studies of the velocity profiles of water flowing through nano-channels showed that with tiny excursions of the wall the slip length becomes independent of the shear rate (Sega, et al. 2013). A characteristic excursion of $\xi = 0.01nm$is defined, below which the correlation exists and beyond which the slip-length is constant. Furthermore, the investigation has shown that thermally conductive, flexible walls increase the slip length due to reduction in friction, while insulating walls show no-slip provided that the excursion is above the aforementioned characteristic value. The roughness of the wall was also studied using a HMCM (Sun, et al. 2012, Asproulis & Drikakis, 2010). The above investigations showed that liquid particles can get trapped in the concaves, resulting in a negative slip which is correlated with the wall separation distance as a power law.

The flow and structure of fluid particles was examined under different channel parameters and under the influence of an external force using a DPD model (Kasiteropoulou, Karakasidis and Liakopoulos 2011). It was observed that the interatomic interactions between the walls and the pseudo-particles result in larger number densities at the solid-liquid interface which in turn results in a greater velocity slip at the boundary, coinciding with previous MD studies. The slip, however, experiences only minor variations as the external force field is increased, even though the average velocity increases. The pressure of the system was found to increase along with the wall-fluid interactions, wall density, cut-off distance and the external force. However, the wall density and external force introduced inhomogeneities in the pressure profile of the channel.

MD simulations have shown that vibrating Carbon Nanotubes (CNT) can act as efficient natural pumps (Qiu, Shen and Guo 2011). The excited state of the CNTs causes the water molecules to flow via centrifugal forces. The water molecules form a continuous array making the method a robust pump. Furthermore, it was shown that even relatively wide nanochannels can initiate a significant amount of mass flow, making the technique a viable option for future applications .Induced flow of water molecules confined between planar surfaces, can also be achieved by placing the system in a rotating electric field (De Luca, et al. 2014). As natural dipoles, the water molecules start spinning, and the torque exerted by the field converts the angular momentum into linear. The principle was tested under realistic environments in which one of the planes is made out of Graphene and one of β-cristobalite, both of which are hydrophobic materials. The collective contribution is that such methods can be used to achieve noncontact pumping of water in nanofluidic scenarios.

A DPD investigation of using confined liquids as natural pumps, focusing on the sensitivity analysis of the electro-osmotic flow (EOF), induced by applying a potential difference across the system, for both Newtonian and non-Newtonian fluids, was published in (Darbandi, Zakeri and Schneider, DPD simulation of electroosmotic flow in nanochannels and the evaluation of effective parameters 2010). The results indicated that the behaviour of the EOF depends largely on the size of the channel, the potential from a point in the fluid due to the effect of the electric double layer (EDL) and the flow index number, describing the shear stress.
Nanoflows have also been considered for the damping of shockwave propagation (Al-Qananwah and Koplik 2013). MD investigations modeled a shockwave colliding onto a solid, with and without a small intermediate porous material in front of it. The results concluded that the stress magnitude and energy deposited in the solid is reduced 30% in the presence of the nanofluidic structure. Additionally, the pores significantly reduce the loading rate.

The use of micro and nano channels for cooling devices requires a deepened understanding of the thermodynamic behaviour of such systems. Studies so far have identified that thermal properties are tightly correlated with the size of the channel. A study of flow through carbon nanotubes (Liu, et al. 2005) identified an anisotropic behavior of the thermal conductivity of such systems, arising from the reduced diffusion coefficient in the direction of confinement. The thermal conductivity in the direction normal to the wall was found to increase with increasing the wall separation distance. The conductance in the parallel direction, however, was found to decrease along with increasing wall separation. This is in contrast with another study which investigated the flow of liquid argon through krypton nanochannels (F. a. Sofos 2009) and found that the thermal conductivity of the liquid increases with increasing wall separation distance, and reaches its bulk value at approximately $20\sigma \approx 7nm$ channel width. Figue 4 shows the MD visualization of liquid argon in a nanochannel.

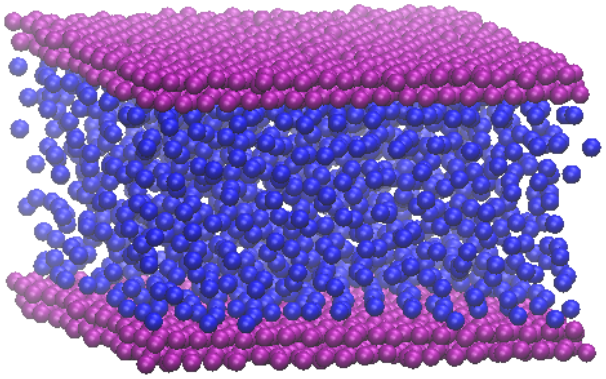

FIG. 4 Visualization of liquid argon in a nanochannel.

Recent studies by the authors focus on thermal diffusion in confined liquids (Frank, et al., 2014a,b). The study found that low density liquids have a greater thermal conductivity than high density liquids, a phenomenon clashing with the conventional understanding of bulk liquids. The density, however, also interferes with the correlation between the heat conductance and the wall separation distance, with low density liquids increasing while high density decreasing as the channel width becomes bigger.

The thermal resistance has been investigated in previous studies and was found to be highly correlated with the theoretical frequency of oscillation of the walls (Kim, Beskok and Cagin 2008). Recent MD simulations (Kio, et al. 2014) have determined a strong correlation between the atomic mass of the walls and the temperature jump at the solid surface. A HMCM study of Kapitza resistance in nano- and micro-channels in the presence of excursions on the walls has found that the thermal resistance increases when increasing the channel height (J. Sun, Y. He, et al. 2012).

4. Concluding remarks

The paper presented a collective overview of modern computational methods used in simulating micro and nano flows. The challenges associated with the modelling of the broad range of physical scales occurring in micro and nanoflows using continuum mechanics were discussed. MD can provide deep insight into the physics of fluid flow and heat transfer but still remains a very expensive approach for using it in practical engineering applications. HMCM and other multiscale methods offer a promising alternative. However, the implementation of these methods, as well as their accuracy and efficiency, is still problem dependent.

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