Hybrid molecular-continuum methods for micro- and nanoscale liquid flows

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Abstract Many flows at microscale and below are characterised by an inherent multiscale nature and accurate numerical modelling of the phenomena involved is the cornerstone for enhancing the applicability of micro and nanofluidics in the industrial environment. This paper presents a hybrid molecular-continuum strategy named as point wise coupling for studying complex micro- and nanoscale flows. In this strategy one performs continuum simulations and uses a molecular solver for computing flow properties. The hybrid methodology utilises a numerical procedure to minimise the cost of the computationally expensive molecular solver. Simulations have been carried out for a slip Poiseuille flow test case. The hybrid results are in good agreement with analytical solutions and pervious molecular simulations.

Keywords: Hybrid Continuum Molecular, Multiscale Modelling, Liquid Slip, Nanofluidics

1. Introduction

During the last decade micro- and nanofluidics have experienced applications in various areas spanning from drug delivery to nano-manufacturing (Kamholz et al., 1999). As an emerging field, the study of flows in micro- and nanoscales is expected to have a great impact in the near future on the design process for a number of high throughput devices (McClain et al., 2003).

The flow characteristics of micro- and nanoscale devices, such as mirco-electro-mechanical systems (MEMS), micro-sensors and micro-reactors, are determined by a high surface-volume ratio which leads to different phenomena than in larger scale devices with similar geometries. Thus, the performance of such devices is particularly sensitive to the surface properties and a better understanding of their influence on the flow physics is of paramount importance for accurate numerical experiments (Gad-El-Hak, 2006). The fluid flow in micro- and nanoscale systems cannot be fully predicted by relying solely on traditional continuum models based on Navier-Stokes with no slip boundary conditions, because of the importance of slip at the surfaces, which increases along with the reduction of the geometrical size. The presence of slip and its magnitude is dependent on the properties, either structural or dynamical, of the solid-liquid interface (Priezjev, 2007a). One approach is to use slip models. However, in cases where the boundary conditions are sensitive to the molecular roughness of the surface and its wetting properties, molecular simulations have to be employed (Liu et al., 2007; Priezjev, 2007a). Molecular simulations are computationally intensive, which restricts their application to nanoscale systems and time scales below microseconds. Thus, modelling flows inside micro- and nanofluidic devices presents a significant challenge due to the inaccuracy of the continuum models and inefficiency of the molecular ones in the meso-scale regimes. To address this challenge, multiscale and specifically hybrid molecular continuum methods have been developed (O'Connell and Thompson, 1995). This type of multiscale methods provides a unified description across a range of time and length scales.

Several multiscale approaches in the hybrid molecular-continuum context have been proposed in the literature over the last years (Kalweit and Drikakis, 2008a; O'Connell and Thompson, 1995; Flekkoy et al., 2000; Delgado-Buscalioni and Coveney 2003;

Werder et al., 2005; Nie et al., 2006; Li et al.,1999; Asproulis, Kalweit and Drikakis, 2008; Hadjiconstantinou and Patera, 1997; Asproulis and Drikakis, 2009). The majority of these methods uses a domain decomposition approach, which is applicable for problems where the continuum model is valid within the majority of the simulation domain, but cannot fully predict the phenomena in a particular geometrically confined area. The natural idea is to decompose the domain into two regions, where the one is modelled using molecular solver and the other through a continuum fluid dynamics (CFD) solver (Kalweit and Drikakis, 2008a; O'Connell and Thompson, 1995). The solution is computed independently in each region and the two descriptions exchange information at specific points in time through a hybrid solution interface (Kalweit and Drikakis, 2008a,b). The benefits by employing the domain decomposition approach are twofold. The continuum solver is not applied in regions where the continuum approximations break down and the computational intensive atomistic simulations are limited to the necessary spatial regions. For any unsteady cases the domain decomposition techniques can not decouple the time scales between the macroscopic and microscopic description. Therefore, the overall computational time is limited to the time scales computable by the microscale solver (Asproulis, Kalweit and Drikakis, 2008; Asproulis, Shapiro, Kalweit and Drikakis, 2008).

The computational limitations of the aforementioned techniques have lead to the development of new multiscale approach named as point wise coupling (PWC) (Asproulis, Kalweit and Drikakis, 2008; Asproulis, Shapiro, Kalweit and Drikakis, 2008). On the contrary to the domain decomposition, in the PWC the microscopic solver is used as local refinement aiming to enhance the accuracy of the continuum solver, and is not applied to a specific initially selected region. The entire domain is modelled macroscopically and the microscale operates as a dynamic feedback mechanism for data required by the continuum solver. An essential characteristic of the PWC is the natural decoupling between the macroscopic and microscopic timescales.

It is ideal for cases, where the characteristic time scales of the flow phenomena are large compared to the microscopic time scales, and therefore from the molecular perspective the flow is a quasi steady state during the continuum time steps at each point of the entire flow field.

This study investigates the application of the PWC as a generic tool to provide boundary conditions for micro- and nanoscale liquid flows over solid surfaces. The outline of the paper is as follows: In Section 2 the PWC methodology and the techniques for exchanging information between the macroscopic and microscopic description are briefly presented. Section 3 discusses the hybrid PWC studies for liquid slip and in Section 4 the conclusions are summarised.

2. Point Wise Coupling Methodology

In the PWC the solution in the entire domain is advanced through the continuum solver and the atomistic models are utilised to:

- Provide accurate boundary conditions such as tangential stress, temperature, or slip velocity
- Substitute constitutive relations, for example, calculate pressure ($P(\rho,T)$)
- Calculate transport properties, such as viscosity for non-Newtonian fluids or thermal conductivity

To that end, the MD solver is engaged to calculate macroscopic quantities at selected points in space and time for the prevailing continuum conditions. In this paper we concentrate on boundary conditions, but the demonstrated techniques can be applied to the other two aspects as well.

One of the challenges of the PWC is to ensure the consistency between the performed MD simulations and the corresponding continuum ones. Therefore, the molecular system is initialised according to the

continuum density, ρ_{con}, and temperature, T_{con}. During the actual atomistic simulations, it is then constrained to the continuum velocity and temperature gradient by controlling the molecular motion within confined regions at the boundary of the molecular domain (Ren and Weinan, 2005; Ren, 2007).

Enforcing the continuum constraints requires altering the properties of the atoms inside the constrained region to match the continuum velocity, $\boldsymbol{u}_{con}$, and temperature, T_{con}. Additionally, the local continuum pressure, P_{con}, must be applied normal on the outer surface of the constrained region in order to keep the atoms within the molecular domain and to subject the molecular system to the correct pressure. For the scope of the current study the examined test cases are liquid flows and, therefore, the continuum state is applied through a periodic re-sampling from a Maxwell-Boltzmann distribution function (Ren and Weinan, 2005; Hadjiconstantinou and Patera, 1997). This technique, when applied to liquid flows (Hadjiconstantinou, 1999a; Asproulis, Kalweit, Shapiro and Drikakis, 2008), provides a computationally elegant mechanism for the continuum information to be transferred in the molecular solver and delivers atomistic results consistent with the applied continuum state.

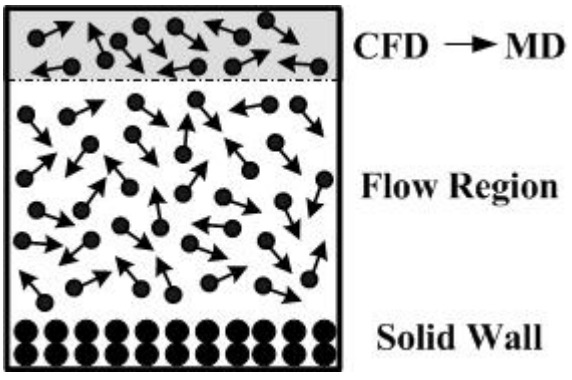

Figure 1. Schematic representation of molecular region in PWC

2.1 Continuum to Molecular

A typical configuration of a molecular domain utilised for PWC simulations is shown in Figure 1. The continuum state is imposed in the upper region. To enforce $\boldsymbol{u}_{con}$ and T_{con} throughout the simulation, the particles' velocities inside that area are periodically drawn from the Maxwell-Boltzmann distribution. The Maxwell-Boltzmann distribution defines the most probable velocity component of an atom, based on its temperature T and mass m. It is the basis of the kinetic theory of gases (Hirschfelder et al., 1964) and corresponds to the natural velocity distribution of an atomic or molecular system in an equilibrium state (Bimalendu, 2002). The probability density $f(\boldsymbol{C})$ of the thermal velocity $C = u/\left(2k_B T/m\right)^{0.5}$ for the Maxwell-Boltzmann distribution is given by

$$f(C) = \frac{1}{\pi^{3/2}} \exp\left(-C^2\right) \quad (1)$$

Each particle in the upper region is assigned with velocity $\boldsymbol{u} = \boldsymbol{u}_{con} + \boldsymbol{u}_{maxwell}$, where $\boldsymbol{u}_{maxwell}$ is the velocity of the Maxwellian distribution and $\boldsymbol{u}_{con}$ is the macroscopic velocity. The assigned atomistic velocities in the constrained region are then defined as

$$u_{i,\alpha} = u_{con,\alpha} + \sqrt{\frac{k_B T_{con}}{m_i}}\psi \quad (2)$$

where ψ denotes a Gaussian distributed number $N(0,1)$ and $u_{con,a}$ is the α^{th} component of the continuum velocity.
In order to ensure that every particle remains inside the molecular domain a reflective plane is placed at the outer boundary of the constrained region.

2.2 Molecular to Continuum

For the test cases of the current study it is the slip velocity at the solid-liquid interface, which is calculated from the molecular simulations and fed back to the macroscopic model. The transfer of information from the molecular to continuum description, although less complicated compared to the reverse procedure, is crucial for the efficiency and accuracy of the hybrid scheme.

In atomistic simulations the calculation of macroscopic variables is performed through

averaging the corresponding microscopic properties. Thus, the information transferred to the continuum description is subject to fluctuations in space and time. The fluctuations can affect the stability and convergence of the continuum solver, which is a problem that primarily concerns the geometrical decomposition approach. For the PWC fluctuations can be reduced simply by increasing the number of atoms and/or the number of time steps from which the respective quantity is calculated. This is achieved by increasing the volume of the cell and the overall simulation time for which the calculations are performed. and is possible through the decoupling of time and length scales in the PWC.

In the first implementation of PWC (Asproulis, Kalweit and Drikakis, 2008; Kalweit et al., 2008) molecular simulations were performed at every time step of the continuum solver. The macroscopic quantities of interest were measured from the MD simulations and fed back to the CFD solver, where they were used to advance the solution in time. This basic procedure leads to repetitive MD simulations of nearly identical states and, thus, a more sophisticated algorithm that utilises already performed MD simulations is employed here. For simplicity consider an example as illustrated in the Figure 1, where the MD simulations of the flow at a wall boundary have to be performed for specified densities, ρ_{con}, and velocities, $u_{con.}$ The slip velocity as function of ρ_{con} and u_{con}, i.e. $u_{slip}(u_{con}, \rho_{con})$, is fed back to the continuum solver. Instead of performing atomistic simulations for every data set required by the continuum solver, the continuum states are discretised based on an initial value, u_{in}, ρ_{in}, and an interval, δu, $\delta\rho$. Therefore, when a set of (u_{con}, ρ_{con}) is given as an input, the discrete sets $(u_{in} + m\delta u, \rho_{in} + n\delta\rho)$, $(u_{in} +(m+1)\delta u, \rho_{in} +n\delta\rho)$, $(u_{in} +m\delta u, \rho_{in} +(n+1)\delta\rho)$ and $(u_{in} +(m+1)\delta u, \rho_{in} +(n+1)\delta\rho)$ are identified, where $u_{in} + m\delta u < u_{con} < u_{in} + (m + 1)\delta u$ and $\rho_{in} + n\delta\rho < \rho_{con} < \rho_{in} + (n + 1)\delta\rho$ and $m, n \in Z$. Molecular simulations are then performed for the four data sets and through a bilinear interpolation the outcomes for the input (u_{con}, ρ_{con}) are calculated. The calculated molecular data are stored and are utilised when another input is in the same or an adjacent interval. Therefore, as the simulation evolves the number of the performed MD simulations is minimised. Furthermore, modifying the parameters δu and $\delta\rho$ determines the number of total atomistic simulations to be performed; larger values imply less MD simulation. This can be used to achieve a balance between accuracy requirements and the available computational resources for a specific simulation.

3. Hybrid Studies of Liquid Slip

In micro and nanofluidic devices, where large surface to volume ratio is present, fluid flow can be significantly affected by the existence of slip in the liquid-solid interface. The most commonly used model for the slip prediction is the Navier boundary condition (Thompson and Troian, 1997) with the slip velocity being proportional to the local shear rate

$$u_{slip} = L_s\dot{\gamma}\,, \quad (3)$$

where u_{slip} is the slip velocity, L_s is a constant slip length and $\dot{\gamma}$ the local shear rate. The application of this model delivers realistic results for a specific flow regime. However, it fails to provide an overall description of the momentum transfer at solid liquid interfaces (Thompson and Troian, 1997). This is due to the fact that the slip length is generally not constant and the non-linear relationship between lip and local shear rate. A number of parameters such as the surface roughness, hydrophobicity and hydrophilicity and the shear rate have great impact on the amount of slip generated. To circumvent the aforementioned issues and increase the modelling accuracy, hybrid PWC simulations were performed, where the slip was calculated from first principles. The chosen test case was a planar Poiseuille flow driven in by an external force f_x in the x direction. A Lennard-

Algorithm 1. PWC- Numerical and Molecular Operations

1. For every input velocity u_{con} find $m \in Z$ where $u_{in} + m\delta u < u_{con} < u_{in} + (m + 1)\delta u$
2. Search in the stored data if simulations with inputs either $u_{in}+m\delta u$ or $u_{in}+(m+1)\delta u$ have been performed
3. If one or more simulations have been previously performed, then run MD for the missing data
4. Store the produced slip velocities, u_{slip}^{m} and/or u_{slip}^{m+1}, in the simulation's data library
5. Based on the library data calculate the slip velocity required by the continuum solver:

$$u_{slip} = u_{slip}^{m} + \frac{u_{slip}^{m+1} - u_{slip}^{m}}{\delta u}\left(u_{con} - \left(u_{in} + m\delta u\right)\right)$$

Jones fluid was used, for which two atoms i and j with the a distance of r_{ij} interact by the LJ-potential

$$V_{ij}^{LJ} = 4\varepsilon\left(\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6} - \left(\frac{\sigma}{r_{c}}\right)^{12} + \left(\frac{\sigma}{r_{c}}\right)^{6}\right), \quad (4)$$

where ε is the characteristic energy level, σ is the molecular length scale and r_c the cut-off distance, beyond which the interactions are neglected. For liquid Argon ε = 120 Kk_B and σ = 0.34 nm (Hadjiconstantinou, 1999b), where k_B is Boltzmann's constant, atomic mass m. The fluid density was $\rho = 0.81\ m\sigma^{-3}$ and the temperature $T = 1.1\ \varepsilon k_B^{-1}$, which corresponds to viscosity $\mu = (2.0 \pm 0.2)\ \varepsilon\ \tau\sigma^{-3}$ (Priezjev, 2007b). The channel height was $H = 2h = 220\sigma$ and the force f_x was investigated in the range of 0.002 to 0.003 ε/σ.

The analytical solution of the Navier-Stokes equation for the slip Poiseuille flow is

$$u(y) = \frac{\rho f_x}{2\mu}\left(h^2 - y^2\right) + u_{slip} \quad (5)$$

Since the density and temperature were constant throughout the simulation domain, the only input parameter for the molecular simulations was the continuum velocity near the boundary solid wall. The MD simulations were performed with $u_{in} = 0.0\sigma/\varepsilon$ and $\delta u = 0.5\sigma/\varepsilon$, which means that molecular simulations were performed only for velocities multiple of 0.5 and the slip for all other input velocities was calculated through interpolation as it is shown in Algorithm 1.

For the PWC scheme MD simulations were performed for the lower and upper walls and provided to the continuum solver the corresponding slip velocity. The size of the atomistic domain was 20σ, 28σ, 10σ in the x, y and z direction respectively, resulting in a total number of 5197 atoms. The continuum velocity was enforced onto the atoms in the region $26\sigma < y < 28\sigma$, whose velocity vectors were drawn every 100 time steps from a Maxwell-Boltzmann distribution according to the u_{con} and T_{con}. The molecular time step was 0.005τ and a total number of $4 \cdot 10^5$ time steps were performed for each simulation. In the molecular simulation, the wall was placed at the lower boundary and modelled by two planes of a face-centred cubic (FCC) lattice with an orientation that forms a (111) surface. The angle between the flow and the orientation of the surface was zero, which in combination with the (111) FCC plane minimises the roughness of the surface and consequently maximises the slip at the boundary. The interatomic interactions of the wall and fluid material were like the fluid modelled by the shifted LJ-potential. The wall density was $\rho = 4.0\ m\sigma^{-3}$ and temperature $T = 1.1\ \varepsilon k_B^{-1}$. Wall-fluid interactions were also modelled by the LJ potential with energy ε_{wf} and length scale σ_{wf} and the parameters used were $\varepsilon_{wf} = 0.4\varepsilon$, $\sigma_{wf} = 0.75\sigma$ as in a similar study by Thompson and Troian, 1997. The heat exchange was controlled by a Langevin thermostat with a random uncorrelated force and a friction term $\Gamma = 1.0\ \tau^{-1}$, where τ is the characteristic time $\tau = (m\sigma^2/\varepsilon)^{1/2}$ (Thompson and Troian, 1997; Yen et al., 2007). The thermostat was only applied in the z-direction to avoid any undesirable influences in the flow direction.

Figure 2 shows the variation of the slip length L_s, as it is calculated from the performed MD simulations as a function of the local shear rate. An interesting feature is that from lower shear rates the slip length presents small variations and is equal to its minimum value $L_{s_0} = 9\sigma$. This is consistent with the Navier boundary conditions; however, for higher shear rates the Navier condition is not valid, since the slip length varies non-linear with the shear rate. A form that has been suggested (Thompson and Troian, 1997) to describe this non-linear relationship is

$$L_s = L_{s_0}\left(1 - \frac{\dot{\gamma}}{\dot{\gamma}_c}\right)^{-0.5} \quad (6)$$

where $\dot{\gamma}_c$ is a critical value at which the L_s diverges. Figure 2 shows good agreement between the data produced from the MD simulations performed in the hybrid framework and Equation 6 which is based on previous molecular studies. Figure 3 shows the velocity profile for a Poiseuille flow with driving force f_x = 0.002 - 0.003 ε/σ as it is calculated from PWC simulations. From Figure 4 one can be identified that the slip velocities are increasing non-linearly as a function of the driving force and consequently the shear rate.

Equations 3, 4 and 6 can be utilized for calculating the slip velocities analytically. Using Equation 3, the shear rate $\dot{\gamma}$ can be determined and can be substituted in Equation 4 to obtain the slip length and consequently the slip velocities. Figure 4 shows the hybrid PWC values of the slip velocities as a function of the driving force towards the analytical values from Equations 3, 4 and 6. Both outcomes are in excellent agreement with small deviations only observable for the minimum and maximum values of the driving force, which can be attributed to measuring errors in the microscopic simulations and the empirical nature of Equation 6, which has been fitted to results of MD simulations in which slightly different potential parameters and/or integration algorithms may have been used.

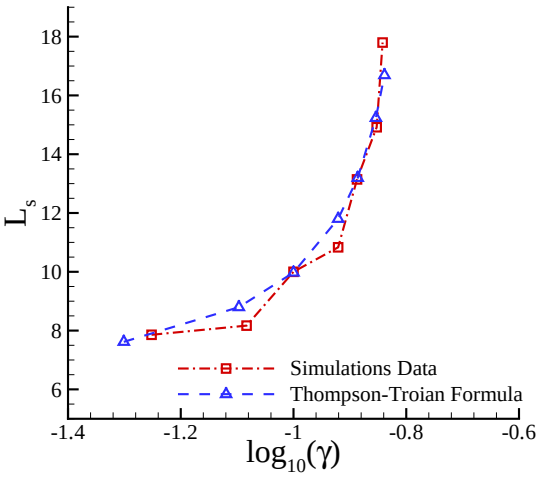

Figure 2. Variation of slip length with the shear rate

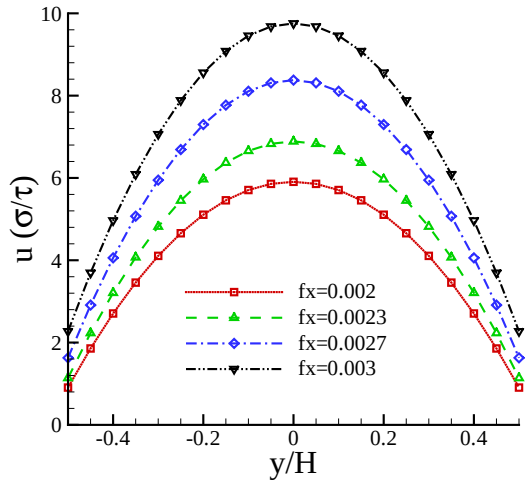

Figure 3. Velocity profiles under different values of the driving force

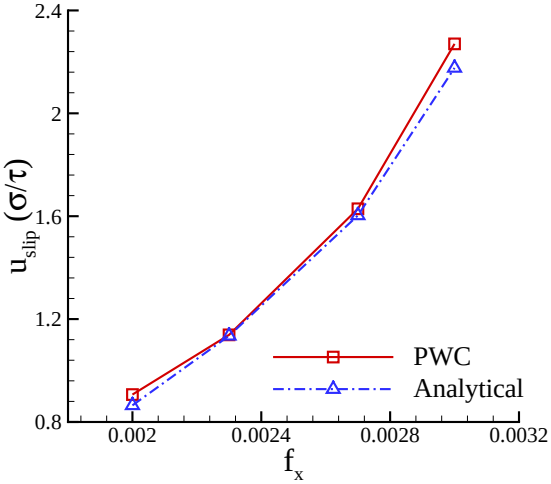

Figure 4. Analytical and computational data of slip velocity as a function of the driving force.

4. Conclusions

In this study a new Point Wise Coupling multiscale method is presented and applied to nanoscale and mesoscale fluid flows with slip at the liquid solid interface. The PWC method effectively decouples the length and timescales. The proposed interpolation scheme utilises the data produced by previous MD simulations through a numerical optimisation procedure. Hence, PWC effectively avoids performing MD simulations for nearly identical continuum states realising an extreme reduction of the method's computational burden. By tuning the interval parameter of the interpolation scheme, for example δu or $\delta \rho$, the number of the performed MD simulations can be regulated to balance between accuracy, stability and efficiency. An open question for following studies is to investigate how the interaction between the continuum and molecular description can impact the convergence and stability of the former and how the PWC with its numerical optimisation procedure can minimise such phenomena.

Despite the fact that the interpolation scheme minimises the number of molecular simulations, the microscopic solver is still the most computationally demanding task of the entire method. The applicability and commercialisation of these methods in the industrial environment requires the development of new versatile strategies to further advance the existing hybrid frameworks.

Acknowledgments

The financial support from EPSRC, MoD and AWE through the grant EP/D051940-JGS 607, as well as from the European Commission under the 6th Framework Program (Project: DINAMICS, NMP4-CT-2007-026804), is greatly acknowledged.

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