Hybrid Molecular Dynamics-Monte Carlo method for heat and flow analysis in micro/nano-channels

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Abstract. We present a hybrid simulation method combining Molecular Dynamics (MD) and Monte Carlo (MC) simulation methods to study properties of fluid flows in micro/nano-channels. The method is used to study a cold gas cooling the warm walls of a micro/nano-channel. Density, flow-velocity and temperature distribution in the channel for different parameters are investigated, and the effect of different wall boundary conditions (hydrophilic/hydrophobic wall interactions) on these results is analyzed by performing pure MD, pure MC and hybrid MD-MC simulations

Keywords: molecular dynamics, monte-carlo, hybrid simulations, heat transfer, micro/nano-channel cooling
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INTRODUCTION

Micro and nano-scale heat transfer is increasingly important in answering fundamental scientific questions and in practical applications. Cooling techniques are examples of such applications playing an essential role in the process of developing and manufacturing of microelectronic components. In the last decade, the trend is that the power consumption of electronic components is increasing with a factor 10 every 6 years [1]. Local high temperatures (hot spots) appear during operation and local cooling is required. As the limits of existing cooling techniques are reached, new micro-scale cooling techniques are urgently needed.

Single and two-phase forced convective flows in micro/nano-channels are such promising techniques for the cooling of electronic devices (e.g., on-chip cooling) ensuring optimal performance and lifetime of these components. Large surface to volume ratio in micro/nano-channels can enhance heat and mass transfer rates. However, on this scale the continuum approach breaks down. For micro-channel cooling, the continuum model for the flow starts to fail when the dimension of these channels is too small or when the gas becomes too dilute [2]. Large amount of heat can be better dissipated through evaporation, but the phase transition from liquid to vapour cannot be described by a continuum approach. New models able to incorporate phase transition are required. Moreover, when the length scale of the fluidic system is reduced, surface phenomena become very important. When catalytic surface activity is present in the micro/nano-channels, temperature control becomes even more difficult. These surface reactions, when exothermic, can contribute to the heat flux and hot spots are generated into the system. In order to predict accurately the heat transfer in micro and nanostructures, the cooling mechanism needs to be investigated on a molecular level.

Refined molecular models are strongly required and particle simulation methods like Molecular Dynamics (MD) and Monte Carlo (MC) have to be applied. MD is a very accurate method able to simulate complex behaviour, but it is computationally very expensive. On the other hand, MC is a stochastic method, able to simulate the bulk properties but with the restriction of less accuracy near the boundaries and not simulating the small scale-effects in the system and phase transitions [3,4,5,6,7,8,9]. Hybrid approaches able to interplay between the simulations of atomistic processes within a small region and the simulation of properties in the bulk, have been previously used, but all these approaches were coupling continuum with either MC or MD [10, 11,12,13,14]. When continuum approach fails [2], hybrid approaches based on particle methods need to be used.

A new hybrid approach coupling MD with a stochastic particles simulation approach [16] based on Monte Carlo (MC) simulation is used here to study heat and flow properties in micro/nano-channels. We first introduce the physical model, then we explain the coupling in the hybrid MD-MC method. Simulation results are validated by comparison with pure MD simulation results of a system consisting of dense gas molecules confined between the walls of a micro/nano-channel. Flow and no-flow regimes are considered for comparisons and the predictions for heat transfer and pressure in micro/nano-channel cooling applications are discussed.

THE PHYSICAL MODEL

Our model to study the one-dimensional heat flow in a micro-channel consists of two parallel plates of length L_y at a distance L_x apart from each other and of gas molecules confined between these two walls. Both plates have their own temperature, T_1 and T_2 respectively, where this temperature is uniform on the plate surface and constant in time. The gas consists of spherical particles of diameter a and mass m, at temperature T. The density of the gas can be expressed as n, being the number of particles per unit of volume, or using a reduced density η, which also takes the particle sizes into account and is related to the number density as $\eta=\pi n a^3/6$ [5]. The mean free path of the gas particles is related to this reduced density. For a relatively dense gas with $\eta \approx 0.1$, the mean free path λ ($\lambda = 1/(\sqrt{2}\pi a^2 nY(\eta))$) and the molecular diameter a have the same order of magnitude. The $Y(\eta)$ factor is the pair correlation function at contact [4,5]. The distance L between the plates, in the x-direction, is always such that both plates are only a few mean free paths apart. For establishing a flow, the particles in the first 3λ are accelerated such that every time step a particle in this region receives an extra velocity in the y-direction of 0.01dt, where dt is the length of the time step. If a particle leaves the channel on the right side, it re-enters the channel on the left with a rescaled velocity according to a lower temperature. In this way the flow is cooled down ($T< T_1, T< T_2$).

HYBRID MOLECULAR DYNAMICS-MONTE CARLO METHODS

In order to perform more efficient simulations, we propose a simulation method that combines the advantages of the Molecular Dynamics and Monte Carlo simulations. How this is done is shown schematically in figure 1 for the case where MD is used in the left half of the simulation domain (regions I and II) and MC in the right half (regions III and IV).

Our simulation algorithm consists of the following steps:

1. First an initial configuration for the whole system is created. The positions of the particles are randomly generated in the simulation domain, and the velocities of the particles are generated from a Maxwell-Boltzmann distribution.

2. The particles in the region in which MD is performed are send to the MD simulator and analogously the particles in the MC range are send to the MC simulator.

3. However, the MD simulation needs information from the neighboring MC particles and vice versa. This is obtained by creating an interface coupling the two subdomains. The MD simulation is extended with a buffer layer (BL_{MD}) to which the information of the MC particles in region III are copied and analogously the MC simulation is extended with a buffer layer (BL_{MC}) to which the information of the MD particles in region II are copied.

4. Now both the MD and the MC simulator can run in parallel. This implies that the MC simulator performs one iteration, updating the positions and velocities of all its particles. Parallel to this, the MD simulator should simulate the same time interval. Because the time step size that can be made in one MD iteration is usually small compared to the time step size in MC, we have to do a number of MD time steps for every single MC simulation step.

5. The information for the whole system is now obtained by recombining regions I and II from MD with regions III and IV from MC. And the simulation can be continued with a new iteration of the hybrid procedure by restarting from step 3.

The first important point is about updating the buffer layers after each iteration of the hybrid method. A straightforward approach is to provide the buffer layers BL_{MD} and BL_{MC} with a new copy of regions III and II respectively. In [15], we have previously investigated the coupling between the two methods in this way that was realized by importing and exporting particles from one simulator to the other. However, as we couple two simulation methods based on a different mechanism of computing the interactions between particles, problems are encountered as expected when trying to couple the less detailed method with the more accurate method. This is the case for coupling the MC and MD particle domains. Whereas for MD to MC particle coupling, particles from the MD domain can be imported directly into the MC domain using the exact positions and velocities, this cannot be done for MC to MD particle coupling as in MC simulations particles can overlap each other. Imported into the MD domain, this would result in very large forces, leading to a high temperature jump in the interface layer caused by energy conservation problems. An option is to reposition the overlapping particles. A new random position is chosen which is accepted or rejected according to a probability distribution depending on the potential energy of the particle at that new position. However, because this has to be done every iteration an equilibrium MD configuration is never formed.

Here an alternative method is used for the MC to MD coupling, where macroscopic properties are copied instead of single particles. In this method the positions and velocities of the particles in the MD buffer layer BL_{MD} are kept and subsequently scaled to match the macroscopic quantities from MC region III. Our hybrid simulator consists of three components, the MD component for the MD simulations, the MC component for the MC simulations, and an interface component between the first two components, coupling the MD and MC simulations. The MD and MC components are independent, the MD and MC steps being computed by two different independent codes based on an already developed software [20] which were implemented in different programming environments, MC simulator in Fortran77, and the MD one in C. Being independent, the MD and MC components can reside on different computers, and can run in parallel being synchronized and coupled by an interface written in Python.

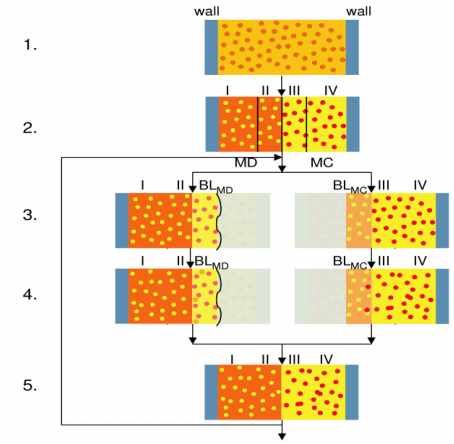


FIGURE 1. The coupling of the MD and MC simulations is obtained via an interface layer. The curved-line boundary of the MD boundary layer BL_{MD} corresponds to the soft (movable) border.

APPLICATION: MICRO/NANO-CHANNEL COOLING

This hybrid method has been used with very good results to simulate systems in the no-flow regime. The results have been validated also by comparisons with pure MD simulation results [16, 18]. In all these simulations thermal wall boundary conditions were used.

This method is extended in order to be able to analyse heat transfer in micro/nano-channels in different flow regimes, and to more accurately simulate the solid-gas interface. A flow is imposed by applying an extra force on particles situated in the first 3λ of the channel. Different MC and MD models can be considered for more accurate gas-surface interactions. In the MD model, the interactions between molecules can be pure repulsive (PR) or attractive repulsive (RA) [17], while in MC different boundary conditions can be imposed (thermal wall, reflective, periodic, etc.).

When thermal wall boundary conditions were used in the no-flow regime, pure MD and pure MC results corresponded very well in the bulk, deviations appearing only in the immediate vicinity of the wall. When the walls are explicitly introduced in the simulations, the discrepancies appear even between different pure MD simulations where walls are either attractive (hydrophilic-RA interactions) or repulsive (hydrophobic-PR interactions). In figure 2, for a cold flow imposed between two warm walls of a channel ($T=0.9T_0$, $T_1= T_2 = 1.0T_0$) we see that different model interactions influence the properties in the channel. The physically more realistic RA model predicts more heat transfer than the more simplified PR model. The flow velocity is higher for hydrophobic interactions than for hydrophilic ones (see figure 4). The attraction causes hardly any slip while the repulsion causes a large slip near the

wall and this results in a higher temperature of the gas in case of the attractive than in case of the repulsive. Thus, although the flow rate is smaller, looking at the temperature profiles we see that the amount of heat that can be removed is larger in case of attractive walls because of the better heat transfer over the interface. This shows once again, that the accuracy of the simulation results depends on how accurate we model the interactions between gas and wall molecules and that pure MC is not good enough to describe these effects.

In figure 3 we compare the density, heat flux and pressure in the channel for a cold flow with T=0.9 T_0, where the hot walls are at the temperature T1= T_2 = 1.0T_0 . From the density profiles we notice that more particles stick to the wall in case of the MD simulation profiles. From the figures we notice that the pressure is slightly smaller for MD-RA (around 0.58 [T / λ^3]) than for MD-PR (0.61 [T / λ^3]), and both are smaller than the MC pressure predictions (0.93 [T / λ^3]). The heat flux on the contrary is slightly higher for MD-RA than for MD-PR, while the heat transfer is very high for the MC as particles colliding with the wall are thermalize faster by the wall. We conclude that we can dissipate more heat not only by increasing flow velocity, but also by increasing the gas-surface interactions.

Hybrid simulations can be used to accurately simulate the gas-surface interactions. The method allows interactions with the wall (attractive-repulsive) within flow conditions. Anyway, from the previous figures we notice that the profiles of the MD-PR and MC simulations are very different. To be able to compare the hybrid simulations with MC and MD for complex boundary conditions, we proceed with considering the simple hard-sphere model for the molecules both in MD and in MC, for the flow without cooling. There are two reasons for this validation of the hybrid method in the flow regime. Firstly, because in order to use the hybrid method, the same model for the particles in MC and in MD is desired in order to assess the influence of the boundaries. As particles in MC are hard-sphere, the first test would be to consider also hard-spheres for MD. Secondly, because flow velocity is increasing with epsilon for MD (see figure 4), for a lower epsilon and extra MD layer with high epsilon (hard-sphere like) should be added for coupling the two sub-domains. For simplicity we consider hard-sphere in both MC and MD. When we compare the flow for hard-sphere, we notice again that MC is different from MD in the middle of the channel even for very high epsilon. When going to lower densities, the relative differences decrease. In figure 5a, 5b and 5c we can see this effect when we consider different gas densities, varying from dilute (η=0.01 in figure 5b), to relative dense (for η=0.1 in figure 5a) and very dense gas (for η=0.2 in figure 5c). At lower density, for η=0.01, the MD and MC axial flow velocity will just correspond (figure 5b). At high densities, these differences in the axial flow velocity between MD and MC are caused by the fact that even for hard-sphere molecules, differences appear between the MD and MC densities next to the wall [16]. The MC density peaks are smaller than the MD ones in the oscillation region, and this causes less collision in MC (less energy transferred between the molecules next to the wall boundary).

Hybrid method would thus help to overcome this problem, by simulating collisions using MD near the wall and MC in the middle. In this way the MC molecules could be thermalized properly (MD-like) by the wall. In figure 5c, looking at the hybrid velocity profile for a fully developed flow when the simulation domain was splitted in 15%MD and 85%MC, we notice that this profile has the same slip near the boundaries as the MD and also the same maximum velocity. In the future, coupling more complex MD models with MC near the boundary of the wall is going to be investigated.

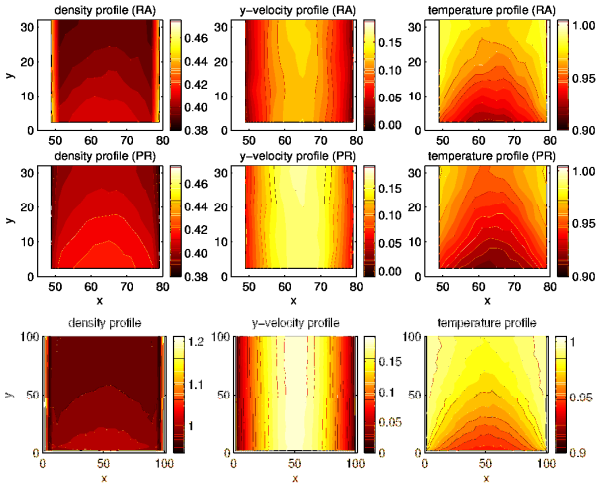
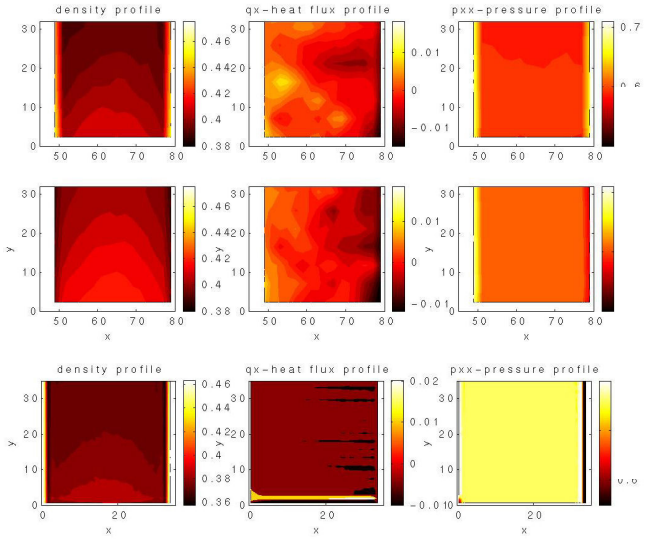


FIGURE 2. Density, flow velocity and temperature distributions in the channels for different sets of interaction parameters, for a cold flow imposed between the two vertical warm walls of the channels: a) MD-RA (repulsive and attractive) interaction between gas and wall particles, b) MD-PR (purely repulsive) interaction between gas and wall particles, c) MC-thermal wall boundary conditions.



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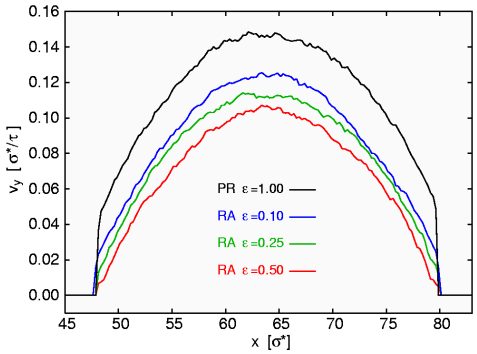
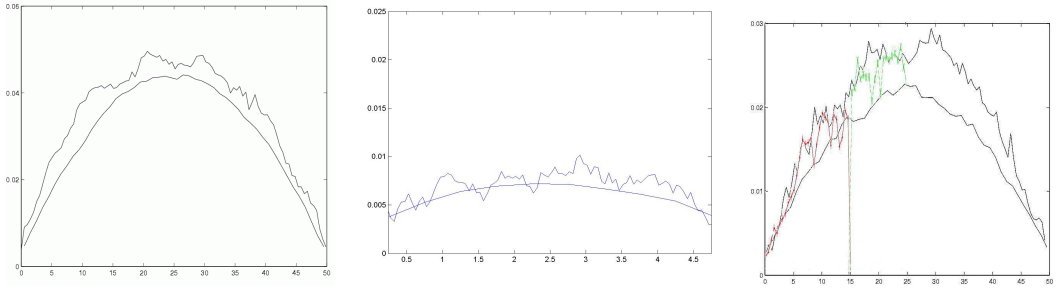


FIGURE 4. Flow velocity for purely repulsive (PR) and repulsive-attractive (RA) gas-wall interaction. Higher velocity profile in case of PR interactions than in case of RA interactions.



a b c

FIGURE 5. Comparison of the axial velocity between MC, MD and hybrid simulations for different densities: a) MD-thermal wall and MC-thermal wall for a fully developed flow profile for η=0.1 (low line-MC, high line-MD), b) MD-thermal wall and MC-thermal wall for a fully developed flow profile for η=0.01 (smooth line-MC, fluctuating line-MD) c) MD-thermal wall, MC-thermal wall (low line-MC, high line-MD) and hybrid–thermal wall for the left side of the channel when 15%MD-85%MC, for η=0.2.

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