# Hybrid Molecular Dynamics-Monte Carlo Simulations for the properties of a dense and dilute hard-sphere gas in a microchannel

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## I. ABSTRACT

We present a hybrid method [8] to study the properties of hard-sphere gas molecules confined between two hard walls of a microchannel. The coupling between Molecular Dynamics(MD) and Monte Carlo(MC) simulations is introduced in order to combine the advantages of the MD and MC simulations, by performing MD near the boundaries for the accuracy of the interactions with the wall, and MC in the bulk because of the low computational cost. The effect of different gas densities, starting from a rarefied gas (reduced density $\eta=\pi n a^3/6=0.001$, where $n$=number density, $a$=molecular diameter) to a dense hard-sphere gas ($\eta=0.25$), is investigated. We characterize the influence of different $\eta$'s and size of molecules on the equilibrium properties of the gas in a microchannel. The effect of the particle size on the simulation results, which is very small in case of a dilute gas, is increasing with $\eta$. Comparisons between MD, MC and hybrid MD-MC simulation results are done, and comparisons between MD, MC, and hybrid MD-MC computational costs are outlined.

## II. INTRODUCTION

In the process of manufacturing and developing microelectronic components, heat management becomes more and more important. The trend is that the power consumption increases with a factor of 10 every 6 years [14]. For ensuring optimal performance and lifetime of these components, new solutions for the cooling will be required. Since local heat sources appear during operation of these devices, local cooling is wanted. Single and two-phase forced convective flows in microchannels become more and more a promising technique for the cooling of such electronic components.

The microchannel cooling represents the most compact and efficient way of transferring heat from a power source to a fluid. Macroscopic models for heat transfer are not sufficient to describe this cooling mechanism in microstructures. The validity of the continuum approach has been identified with the validity of the Navier Stokes equations [3]. This requires the Knudsen number ($Kn = \lambda/L$, where $\lambda$ is the mean free path and $L$ the physical length of the system) to be small compared to unity, the limit being $Kn = 0.1$. When the characteristic size of the device decreases or when the flow is more rarefied ($Kn > 0.1$), the continuum flow model is no longer valid and must be replaced by another model. The governing equations of the flow model must change from the Navier Stokes equations to the Boltzmann equation [3, 6, 7], which involves the molecular velocities instead of the macroscopic quantities. To solve this integro-differential equation for the velocity distribution function using conventional finite element or finite difference methods is difficult since the number of independent variables include both those of physical space and those of the velocity space. The alternative is to use a molecular model where the volume is filled with a large number of discrete molecules and to apply different particle simulation methods to solve the Boltzmann equation taking into account the molecular structure of gases.

The particle simulation methods we use are Molecular Dynamics (MD) [5] and Direct Simulation Monte Carlo method (DSMC) [1–3, 9]. In MD, molecules can move and collide according to the forces the particles exert on each other. In DSMC, movements and collisions of particles occur between large particles concentrating a cluster of real molecules where the collisions are stochastic. For simulating a dense gas flow in a microchannel, the MD method is very time consuming.

For a dense gas the governing equation of the flow model is an extension of the Boltzmann equation, called the Enskog equation [4, 15]. Different MC particle simulation methods have been proposed to solve this equation. The first method described by Garcia [1, 2] is an attempt to bring into DSMC [3] the spatial correlations which are absent in an ideal gas. This method encounters problems with boundary conditions when walls are introduced. A particle method for the numerical solution of the Enskog equation has been presented by Montanero and Santos [10, 11] extending the scheme originally proposed by Nanbu [12] for the Boltzmann equation. The method correctly reproduced the transport

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14. ABSTRACT

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properties of the Enskog gas, but inherited from the original Nanbu scheme the feature of conserving momentum and energy only in a statistical way and not in a single collision. The particle method proposed by Frezzotti [7] constructed for the Enskog equation in the spirit of the DSMC method exactly conserves momentum and energy. We use this latter method for our MC results.

In this paper we present a hybrid method [8] to combine the advantages of the MD and MC simulations, performing MD near the boundaries for the accuracy of the interactions with the wall, and MC in the bulk because of the low computational costs. Using this method, the properties of hard-sphere gas molecules confined between two-hard walls of a microchannel are studied.

In section III, this model of a microchannel is described, followed by a description of MC, MD and our hybrid MD-MC simulation methods. Our goal is to use our MD-MC simulations to study heat-transfer in micro- and nanochannels using different gas densities. For computational reasons we consider nanochannels for our simulation results, such that the walls are separated only by a few mean free paths.

In section IV, simulation results of our hybrid method are presented for different densities, from a dilute to a dense gas. Using the MD-MC simulations, our goal is to study the heat transfer in microchannels using different densities. Comparisons between MD, MC and hybrid MD-MC simulations are done. In the end, comparisons with MD and MC computational costs are outlined.

## III. THEORY

We give the theoretical background for the numerical and simulation results. First we specify our model and then we simulate our system using MC, MD and hybrid MD-MC simulation methods. We describe the methods used for our simulation results. For the hybrid simulation method we describe the algorithm obtained by coupling MD and MC simulations having the same size of simulation particles.

### A. The physical model

The model for the one-dimensional heat flow in a microchannel consists of two infinite parallel plates kept at different temperature and the gas molecules that are confined between these two walls. The gas molecules are modelled as hard-spheres. In these channels, for a relatively dense gas ($\eta \approx 0.1$), the mean free path ($\lambda$) and the molecular diameter ($a$) have the same order of magnitude. The temperature is uniform on the plate surfaces and constant in time. Since the plates are only a few mean free paths apart, the fluid motion is governed by the Enskog kinetic equation [4], as an extension of the Boltzmann equation to dense fluids. This model was proposed by Frezzotti [6, 7] to study the one-dimensional steady heat flow in a dense hard sphere gas. The Enskog equation has the form:

$$\frac{\partial F}{\partial t} + \xi \circ \bigtriangledown F = J_E(F, F), \tag{1}$$

where $F(x, \xi, t)$ is the one-particle distribution function of the molecular velocity $\xi$. The collision integral $J_E(F, F)$ keeps the same binary structure of the corresponding Boltzmann term, but the colliding molecules occupy different positions in space and the collision frequency is modified by the factor $Y$ which plays the role of an approximate pair correlation function. The $Y$ function has the form: $Y(n) = \frac{1}{2}\frac{2-\eta}{(1-\eta)^3}$, where $\eta$ is the reduced density ($\eta = \pi a^3 n/6$), $n$ is the number density and $a$ the molecular diameter.

### B. Monte Carlo Methods

We solve the Enskog equation numerically by means of a particle simulation method. We are looking at the density and temperature profiles of a dense gas in equilibrium near a hard wall. A particle scheme for the numerical solution of the Enskog equation was proposed by Frezzotti in 1997 [6, 7]. In this particle simulation method the molecules of the fluid are replaced by a number of mathematical particles. Each particle is characterized by its position $x$ and its velocity $V$. The particles are allowed to move in the flowfield region and to collide, the collision partners are selected from prescribed collision probabilities. First the particles are advected with their velocities and then collisions take place at each spatial location by dividing the domain into cells. In the case of the Boltzmann equation collisions are computed locally between particles belonging to the same cell. In case of the Enskog equation, because of the finite extent of a molecule, the particles in a given cell can interact with particles located in nearby cells.

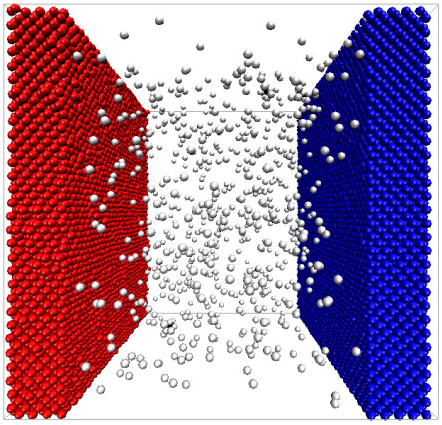

FIG. 1: The gas molecules(black) confined between two walls kept at different temperature. Left: the warm wall($T_1 = 240K$); right: the cold wall($T_2 = 120K$).

### C. Molecular Dynamics

In a MD simulation the motion of the particles is calculated by computing all the forces exerted upon the individual particles. The interactions between particles are described using Lennard-Jones potentials. In order to simulate hard-sphere interactions using MD, truncated shifted Lennard Jones (LJ) potentials were used for the interactions between gas molecules. This basically means that only the repelling part of the LJ potential is taken into account, such that all the interactions between particles situated at distances larger than a cut off radius $r_c = 1.1222 * a$ are ignored. Our MD model for the microchannel, using LJ potential to model the interaction of the molecules, consists of two walls, each consisting of 10 layers of molecules: one cold wall (right wall in figure 1) and one warm wall (left). We are using reduced units in our MD simulations, such that one simulation shows the behavior of multiple systems. For instance, heavier particles will move slower at the same $T$, but one particle at $T$ behave the same as heavier particle at higher $T$. There are three parameters that can be set: the size of the particles ($a$), mass($m$), and unit of energy($\epsilon$). LJ potentials are used to simulate the interaction of the particles in the solid walls. The interactions between wall-gas and gas-gas are modeled by a truncated shifted LJ potential. For the interactions of the molecules in the solid, the standard LJ potential is used with a quite large $\epsilon$ in order to keep the structure of the solid such that it will not mix with gas molecules. A dense Argon gas is considered for the MD simulations, where $a = 0.191nm$, the mean free path $\lambda = 0.346nm$, and initial uniform particle density $n_0 = 3.43$ particles nm$^{-3}$.

### D. Hybrid Molecular Dynamics-Monte Carlo Methods

In figure 2 we notice that the density profiles for both MC and MD have the same shape, differences appear in the peak region as an effect of the different collision mechanisms and of the averaging over more steps in MC. The effect of the particle size on the simulation results is increasing with $\eta$, and it is very small in case of a dilute gas. The effect of different gas densities, starting from a rarefied gas ($\eta = 0.001$) to a dense hard-sphere gas ($\eta = 0.25$), is shown in figure 3.

For relatively dense gases ($\eta > 0.1$), density oscillations and temperature jumps occur near the walls of the microchannel. According to Frezzotti [6, 7, 13] this can be explained taking into account that when the distance of a molecule from the wall is less than the molecular diameter $a$, then a portion of its surface is protected from collisions since there is no room for a collision partner. The molecule is therefore pushed against the wall, which explains the high density of the molecules near the hard wall.

In order to perform more efficient simulations, we propose a simulation method that combines the advantages of the Molecular Dynamics and Monte Carlo simulations, by simulating particles near the wall over the scale of the oscillation region using Molecular Dynamics techniques to obtain more accurate results near the wall, and Monte Carlo techniques for the particles in the bulk to keep the computational cost as low as possible. This is achieved

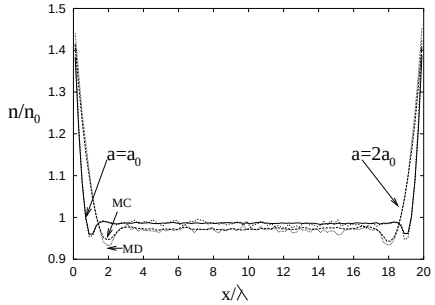


FIG. 2: Comparison between MD and MC density profiles $n/n_0$ for $\eta = 0.1$, $T = 120K$, $n_0 = 3.43$ particles nm$^{-3}$, when $a = a_0$ and $a = 2a_0$.

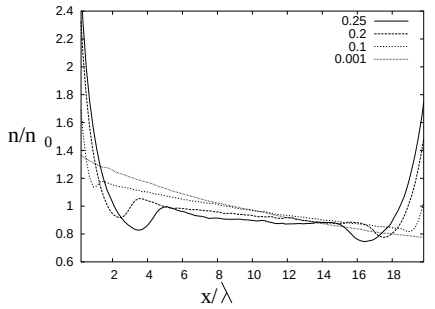


FIG. 3: Density profiles for $\eta = 0.001, 0.1, 0.2, 0.25.$, $T_1/T_2$=2

by dividing our simulation domain into subdomains, one for MD and one for MC. Because the MD method needs information from the neighboring MC particles and vice versa, an interface coupling the two subdomains is built as shown in figure 4.

In order to get accurate results near the wall, a detailed model is needed in which the particles diameter in MC is equal with the molecular diameter of particles in MD. Our hybrid simulation method couples the MD and MC simulations through a buffer layer at the interface between the two domains. In figure 4 we have labelled with (II) the buffer layer of MC subdomain (III+IV), and with (III) the buffer layer of the MD subdomain (I+II).

Our simulation algorithm consists of the following steps:

1. generate initial configuration of the particles in the whole domain.
2. assign particles in region I and II to MD code, and in III and IV to MC code.
3. send properties of particles in region II to MC code, and of particles in region III to MD code.
4. MD simulations of particles in I and II, and MC simulations in III and IV, computing their new positions and velocities.
5. start from step 3.

Initially, the position of the particles are randomly generated in the simulation domain, and the velocities of the particles are generated from a Maxwell-Boltzmann distribution. MC and MD simulations are updating the velocities and positions of the particles assigned to their domain in parallel. Because the time step in MD is normally small compared to the time step in MC, we have to do a number of MD time steps for every single MC simulation step. The average distance travelled by the MC particles between two collisions (mean free path=$\lambda$) is covered by the MD particles over a number of MD time steps. For the case when $\eta = 0.1$ ($\lambda \approx a$), we have used five MD steps and one MC step per iteration. The buffer layer of each subdomain consists of a copy of the boundary layer of molecules belonging to the neighboring subdomain(see figure 4). The particles in the buffer layer are used in the process of computing the new positions and velocities of the particles from each subdomain. This is done in the MD subdomain by computing the interaction forces between particles and updating the velocities and positions solving Newton's equations of motion. In the MC, the collisions between random pairs are computed stochastically, with scattering rates and postcollision velocity distribution derived from the kinetic theory of the dilute gas. Particles are advected

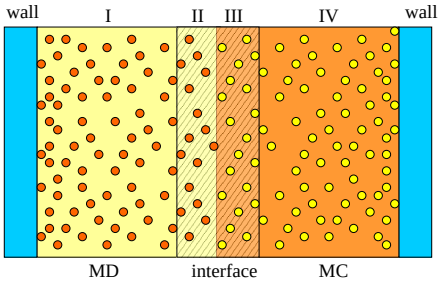


FIG. 4: Coupling of the MD and MC simulations of particles of the whole domain, through an interface layer.

according to these new velocities.

A straightforward approach to update particles in the interface layer after each iteration, is by allowing each subdomain to communicate its own new positions and velocities to the other subdomain. The coupling between two methods can thus be realized by importing and exporting particles from one subdomain to another. As we couple two simulation methods based on a different mechanism of computing the interactions between particles, problems appear 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 particles domains. As for MD to MC particle coupling, particles from the MD domain could be directly imported into the MC domain using the exact position and velocities, this can not 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 high temperature jump in the interface layer for overlapping particles or for particles placed too close to each other. Moreover, problems with energy conservation are encountered. Thus, for the MC to MD coupling, the MD boundary layer (III) is divided into subcells, and the average properties of the particles in the subcells are imported from the MC domain rather than updating the exact positions and molecular velocities.

To update the temperature in the boundary layer (III), particle velocities are rescaled according to the corresponding imported MC average temperature per subcell. Updating the density in the buffer layer (III) is more difficult because of the problems encountered with energy conservation when generating or removing particles in the MD subdomain. Thus, we introduce a soft border for the MD boundary layer (III), such that this border is shifted to the right if the density is decreasing and to the left if the density is increasing. Only in case the density gradient is very high, particles are added or removed from the domain to obtain the required density in the boundary layer.

For the MD to MC coupling, MD particle velocities and positions can be directly imported from the MD and updated in the boundary layer (II). The size of the boundary layer is usually around a few mean free paths. For the MD subdomain, the soft border of the buffer layer can increase or decrease the size of the subdomain with almost a mean free path.

Next we will present our hybrid MD-MC simulation results.

## IV. RESULTS AND DISCUSSION

### A. Comparison between MD, MC, and Hybrid MD-MC results

Initially, we have splitted our domain equally into two subdomains, half of the domain being the MD subdomain, and the other half the MC subdomain like in figure 4. The temperature of the warm wall $T_1$ is twice the temperature of the cold wall $T_2$. Figure 5 shows the hybrid MD-MC simulation results for the density and temperature profile in the channel when $L = 20\lambda$, $T_1/T_2 = 2$, both for a dense ($\eta = 0.1$) and for a more dilute gas ($\eta = 0.01$).

Our simulations profiles are equal to pure MD and pure MC simulation results, proving that we can use the hybrid method to couple MD and MC simulations. The next step is then to use MD near both channel walls and MC in the middle for the bulk. Figure 6 shows the density and temperature profiles in the channel for such a simulation, for the case when both walls and the gas are at the same temperature $T$.

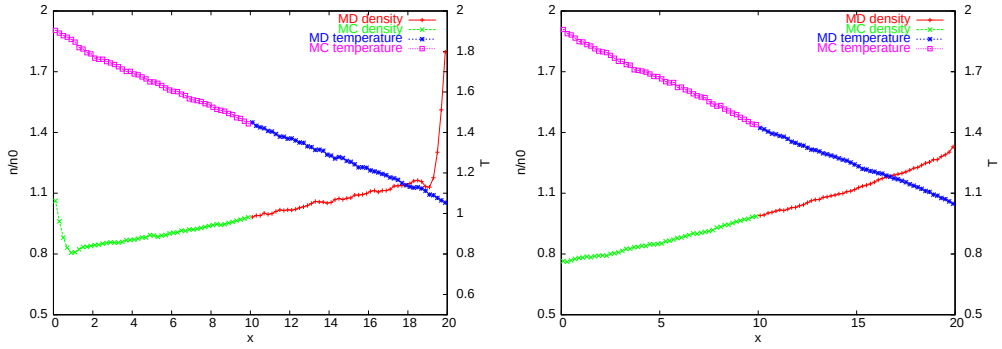


FIG. 5: Hybrid MD-MC simulations for the density and temperature profile in the channel when $\eta = 0.1$(a), $\eta = 0.01$(b), $T_1/T_2 = 2$, $L = 20\lambda$. The domain is splitted in two subdomains, the left one being MC(50%), and the right one MD(50%).

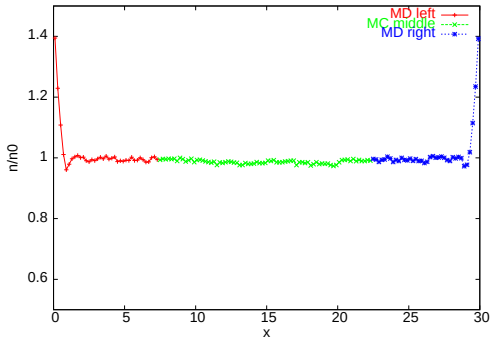


FIG. 6: Hybrid MD-MC simulations for the density and temperature profile in the channel when $\eta = 0.1$, $T_1/T_2 = 1$, $L = 20\lambda$. The domain is splitted into three parts, two MD domains(25%) near the walls and one MC domain(50%) in the middle.

### B. Comparison of simulation times for the MD, MC, and Hybrid MD-MC methods

We have computed the simulation times for the system consisting of 20000 particles. Comparisons between pure MD, pure MC and hybrid MD-MC simulations times were performed for simulations consisting of 500 combined MD-MC iterations, and for different reduced densities ($\eta = 0.1$, $\eta = 0.01$). For a dense gas ($\eta = 0.1$), the 500 combined iterations consisted of 500 MC steps and 2500 MD steps, while for a dilute gas ($\eta = 0.01$) these iterations consisted of 500 MC steps and 30000 MD steps, because 60 MD steps are needed for every MC iteration. For the coupled MD-MC simulations, two situations were considered. In the first case the simulation domain is equally divided between MD and MC. In the second case the MD domain is only 10% of the whole domain containing the region situated near the wall, and 90% is the MC domain in the bulk. The timing results are presented in Table 1. We notice that the speedup when using hybrid MD-MC method for 50% MD and 50% MC is very small when compared to pure MD simulations times, but it increases drastically when the bulk is larger than the region near the wall. For example, when the MC domain is extended to 90% of the simulation domain and MD domain reduced to 10% of the simulation domain, the speedup of the simulations increases with a factor five.

| timings | $\eta = 0.1$ | $\eta = 0.01$ |
|---|---|---|
| pure MC | 2.4 | 2.3 |
| pure MD | 203.3 | 1169.6 |
| MD(50%)-MC(50%) | 246.5 | 1162.9 |
| MD(10%)-MC(90%) | 43.4 | 206.9 |

TABLE I: Simulation times for 500 combined iterations and 20000 particles. For $\eta = 0.1$, simulation times are computed for 500 MC steps and 2500 MD steps. For ($\eta = 0.01$), timings are done for 500 MC steps and 30000 MD steps.

## V. CONCLUSIONS

By coupling different simulation methods we can combine in one hybrid method the advantages of these simulation methods. We have coupled two particle simulation methods, namely Molecular Dynamics and Direct Simulations Monte Carlo. With the hybrid MD-MC approach we are able to study the density and temperature profiles for a dilute and dense hard-sphere gas in micro- and nanochannels. Comparisons between MD, MC and hybrid MD-MC simulations show that our simulation profiles are correct, both for a dilute and a dense gas. For the simulation of gas properties in microchannels, we use combined simulations, doing MD near the walls and MC simulations in the bulk. Comparisons between simulation times using pure MC, pure MD and hybrid MC-MD methods have been given. The results show that the speedup when using 50% of the domain for MD simulations and 50% for MC simulations is very small compared to pure MD simulations times, but it increases drastically for more realistic situations where the region near the wall is small compared to the bulk.

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