HEAT TRANSFER BETWEEN WALLS AND FLUIDS: MD SIMULATIONS WITH VIBRATING WALLS

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ABSTRACT

In Molecular Dynamics simulations of micro channels, a lot of computation time is used to simulate the channel walls when the wall molecules are explicitly simulated. To save computation time, implicit boundary conditions such as the Maxwell conditions can be used. With these boundary conditions, heat transfer is still a problem. In this work, we derive a new boundary condition, based on a vibrating potential wall. The heat transfer properties of the new boundary condition are shown to be comparable to the explicit wall. The computation time needed for the implicit boundary condition is very small compared to the explicit simulation.

1. INTRODUCTION

Last decades computer chips have become more powerful and smaller in size at the same time [1]. As a direct consequence of this technological improvement, the heat per area produced by a computer chip has increased, and is expected to increase further [2]. The conventional way to remove this heat is by air cooling, but the limits of air cooling are being reached.

Micro channel cooling is a promising way to solve the cooling problem for computer chips. In micro channel cooling, a fluid is flowing through a micro channel in close contact with the computer chip. Due to the large area to volume ratio of the micro channel, the heat removal is larger than by conventional air cooling. Heat transfer by forced convection for gases is in the range 25 – 250 kW/m² [3], whereas experimental micro channels with water have shown a heat flux of 500 kW/m² [4]. The heat removal is optimal when evaporation takes place in the micro channel [5]. To optimize micro channel configurations, the heat and flow problems in the micro channel need to be understood, including the heat transfer between the channel wall and the fluid. Because the heat removal by evaporation is large, evaporation should be included in the model.

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Because of the small size of the micro channel, the continuum approximation is not valid in the gas phase [6]. This means that evaporation, an important contributor to the heat removal, can not be analyzed with continuum techniques. Other techniques, that include the particle nature of the fluids should be used to study the process of evaporation and condensation in the micro channel. One of these methods is Molecular Dynamics (MD) [7, 8]. In MD, the trajectories of all particles are calculated by analyzing the interactions between all particles. It is possible to explicitly include wall particles in the MD simulation. Explicit walls are expected to give the best results, but at the price of high computational costs. Because several layers in the wall need to be calculated, the number of particles in the wall can be larger than the number of particles in the fluid, so the majority of the computation time is needed for the simulation of the wall particles.

A solution to the computation time problem in the simulation of explicit walls is fixing the position of the wall particles and only simulating their influence on fluid particles. Although this is time-saving, there is no energy exchange from the fluid particles to the wall particles, so heat transfer between the wall and the fluid is impossible. Because heat transfer between wall and fluid is crucial for micro channel analysis, this method can not be used.

To replace the explicit wall with a computationally less expensive method that is capable of heat transfer, a boundary condition originating from vibrating walls has been derived. In previous work [9], we have shown that this boundary condition gives results in heat transfer between gas and wall that agree with results for an explicit wall, in greatly reduced computation time. In this work, we show how to generalize this result to a boundary condition for MD simulation that allows for heat transfer between fluid and wall.

2. THEORY

2.1 Wall as rigid body

Suppose that a particle is at distance \( x \) from a wall at position \( 0 \), moving towards a wall described by wall potential \( V(x) \). Only \( x \), the coordinate perpendicular to the wall is of interest here. The interaction between the particle and the wall can be described with Molecular Dynamics (MD) [7, 8]. In MD, the motion of particles is simulated, dealing with the interactions by means of a force between particles that is derived from their potential energy \( V \). MD can be used to simulate a system of wall particles and a fluid particle, as shown in Figure 1. The wall particles, positioned in an \( fcc \)-lattice, are vibrating due to their thermal motion. Because of the computational effort needed to simulate this thermal motion, methods have been developed that replace the explicit wall by a computationally cheaper solution. The Maxwell model [10] is a commonly used model, but the accommodation coefficient in that model is not a priori known [11]. We follow a different approach here, in which a particle moving towards a wall interacts with a small part of the wall, as if the wall particles are seen as one rigid vibrating body, shown in Figure 2. The interacting part of the wall is vibrating as if it is connected with a spring with spring constant \( k_w \). In normal situations, the spring constant is in the order of \( 300 \epsilon / \sigma^2 \) [12],

![Figure 1](image1.png)

**Figure 1**: Interaction between a particle and an explicit wall. Inside the wall, all interactions are calculated, and all particles can have different velocities.
where $\varepsilon$ is the typical energy of a particle, and $\sigma$ is the molecular diameter[13]. Because the wall energy $E_w$ (the potential and kinetic energy of the interacting part of the wall) is in the order of $\varepsilon$, this means that the amplitude of the vibration is a lot smaller than a molecular diameter.

### 2.2 Wall motion and particle motion

In Molecular Dynamics the interaction between particles is specified by a potential energy function, giving the potential energy $V$ due to the interaction of two particles at distance $r$. A commonly used potential energy function is the Lennard-Jones potential [7, 8, 14], given as

$$V(r) = 4\varepsilon \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right),$$

where $\varepsilon$ is again a typical energy, and $\sigma$ is the molecular diameter; $\varepsilon$ and $\sigma$ together with the mass $m$ determine the type of molecule. From these constants, a time scale $t_0 = \sqrt{m/\varepsilon \sigma^2}$ can be found. The force between the two particles $F$ is given as

$$F = -\frac{dV}{dr} = -V'(r).$$

Newton’s second laws says that the differential equation for the position of the particle $x$ is given by

$$\frac{d^2x}{dt^2} = -\frac{V'(x-y)}{m},$$

where $m$ is the mass of the particle. The motion of the wall $y$ is determined by the force between the wall and the particle, and the force of the spring. If the spring has spring constant $k_w$, then the differential equation for the position of the wall $y$ is given by

$$\frac{d^2y}{dt^2} = \frac{V'(x-y) - k_w y}{M},$$

where $M$ is the mass of the part of the wall involved in the interaction. This effectively means that the part of the wall involved in the interaction is seen as one bigger and heavier wall particle. The first right-hand term corresponds to the fluid-wall interaction and the second to the spring-wall interaction. The initial conditions are given as

$$x[0] = x_0, \quad x'[0] = v, \quad \frac{k_w}{2} y[0]^2 + \frac{M}{2} y'[0]^2 = E_w, \quad y[0] = \sqrt{\frac{2E_w}{k_w}} \cos(\Phi),$$

where $\Phi$ is the initial phase of the wall, $0 \leq \Phi < 2\pi$. These equations were solved numerically in a one-dimensional Molecular Dynamics simulation using the leap-frog algorithm [8]. The result for initial conditions $x_0 = 1.5\sigma$, $v = 5\sigma/t_0$, $E_w = \varepsilon$ and various initial phases of the wall $\Phi$ is shown in Figure 3. Figure 3 also shows the solution for a non-vibrating wall. If a particle hits a non-vibrating wall, no energy is exchanged: the outgoing velocity is equal to the incoming velocity. The solution where the particle hits a vibrating wall clearly shows lower outgoing velocities; this shows that during the interaction, energy was transferred from the particle to the wall. Another thing that is seen in Figure 3 is that different phases of the wall can result in a different energy exchange. Since we are interested in the average behavior of the particles, the mean exchanged energy $DE$ is analyzed here.
3. ENERGY EXCHANGE

From a dimensional analysis of the problem, three dimensionless parameters can be extracted:

\[ \delta = \sqrt{\frac{2E_w}{k_w \sigma^2}}, \quad \lambda = \frac{1/2mv_0^2 + V(x_0)}{k_BT_w}, \quad \text{and} \quad \mu = \frac{M}{m}. \]  

Here, \( \delta \) can be interpreted as the dimensionless wall amplitude directly related to the temperature, \( \lambda \) is the ratio of energies of the particle and the wall, and \( \mu \) is the mass ratio between the particle and the part of the wall that is involved in the interaction. From literature [15], a value of \( \mu = 3.6 \) is shown to be reasonable in similar problems, and is assumed here also. The total energy of the particle \( E_p \) (kinetic and potential) is a function of these three dimensionless parameters \( \delta, \lambda \) and \( \mu \), the initial phase of the wall \( \Phi \) and the time \( t \), so

\[ E_p = E_p(t; \delta, \lambda, \mu, \Phi). \]  

The mean exchanged energy during a collision is defined as the difference between the total energy of the particle before and after the collision, averaged over the initial wall phases \( \Phi \), so

\[ DE(\delta, \lambda, \mu) = \frac{1}{2\pi} \int_0^{2\pi} \left( E_p(t_0; \delta, \lambda, \mu, \Phi) - E_p(t_1; \delta, \lambda, \mu, \Phi) \right) d\Phi, \]

where \( t_0 \) is a time before the collision and \( t_1 \) is a time directly after the first collision. After the first collision between a fluid particle and an explicit wall, internal wall vibrations will influence the outer wall behavior and the model in Section 2.2 will not be accurate anymore, so the collisions after the first are ignored. Here, a linear approximation of the exchanged energy in \( \delta \) and \( \lambda \) will be used,

\[ DE(\delta, \lambda, \mu) \approx DE(\delta_0, 0, \mu) + \left[ \frac{\partial DE}{\partial \delta} \right]_{\lambda} (\delta - \delta_0) + \left[ \frac{\partial DE}{\partial \lambda} \right]_{\delta} \lambda, \]

with \( \left[ \frac{\partial DE}{\partial \delta} \right]_{\lambda} \) and \( \left[ \frac{\partial DE}{\partial \lambda} \right]_{\delta} \) constant. Here, \( \delta_0 \) corresponds to the dimensionless wall amplitude corresponding to a typical temperature of the problem, and \( \lambda = 0 \) corresponds to a particle that almost escapes from the wall.
In the new approach, equation (9) is taken as a starting point. In the exact situation, shown in Figure 3, a particle close to the wall interacts over a short period of time with the wall, with an energy change that depends on the phase of the wall $\Phi$. In the new model, shown in Figure 4, the particle is not influenced by the presence of the wall until it crosses the ‘interaction boundary’ of the wall. At that moment, the energy exchange according to (9) takes place, and the particle reverses its direction. The ‘interaction boundary’, found from examining situations as shown in Figure 3, is put at $0.8\sigma$ from the wall. This is approximately the distance at which the kinetic energy from the particle is completely changed into potential energy, adjusted for the small distance that the wall moves. This distance is slightly dependent on the energy of the particle, but this small influence is ignored in the analysis, as it will not influence the results much. Hence, the distance of $0.8\sigma$ is used for all interactions.

![Figure 4](image_url)

**Figure 4**: The new model, based on Figure 3. A particle moving towards the wall, is not influenced by the wall until it crosses the interaction boundary, at a distance of $0.8\sigma$ of the wall. At that moment energy is exchanged according to (17), and the particle is reflected with the velocity according to the new energy.

In this boundary condition, three parameters have to be specified: $DE(\delta_0, 0, \mu)$, $\left[\frac{\partial DE}{\partial \delta}\right]_{\lambda}$ and $\left[\frac{\partial DE}{\partial \lambda}\right]_{\delta}$. Two of them are found by analyzing the situation of an ideal gas in contact with the boundary condition. In the model shown in Figure 4, the potential energy contribution from the wall is neglected, so the dimensionless parameter $\lambda$ is

$$\lambda = \frac{E_{\text{kin}}}{k_B T},$$

where $E_{\text{kin}}$ is the kinetic energy of the particle. The kinetic energy $E_{\text{kin}} = 1/2 \, m v^2$ of an ideal gas particle with temperature $T$ passing through a plane, normal to that plane is distributed according to [16]

$$p(E_{\text{kin}}) = \frac{1}{k_B T} \exp\left(\frac{-E_{\text{kin}}}{k_B T}\right),$$

where $k_B$ is again Boltzmann’s constant. With this distribution, the expected energy exchange $E[DE]$ between a wall with temperature $T$ and an ideal gas with temperature $T$ is

$$E[DE] = \int_0^\infty DE(E_{\text{kin}})p(E_{\text{kin}})dE_{\text{kin}} = DE(\delta_0, 0, \mu) + \left[\frac{\partial DE}{\partial \delta}\right]_{\lambda} (\delta - \delta_0) + \left[\frac{\partial DE}{\partial \lambda}\right]_{\delta},$$

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where the latter term was found using the integral outcome
\[ \int_{0}^{\infty} z \exp(-z) dz = 1. \]  

(13)

If the wall and the gas have the same temperature \( T \), on average no heat is exchanged [17], so \( E[DE] = 0 \). This holds for every value of \( \delta \), so
\[
\left[ \frac{\partial DE}{\partial \delta} \right]_\lambda = 0, \quad DE(\delta_0, 0, \mu) = - \left[ \frac{\partial DE}{\partial \lambda} \right]_\delta.
\]

(14)

This means that \( DE \) is independent from \( \delta \), and (9) becomes
\[
DE(\delta, \lambda, \mu) = (\lambda - 1) \left[ \frac{\partial DE}{\partial \lambda} \right]_\delta.
\]

(15)

The coefficient \( \left[ \frac{\partial DE}{\partial \lambda} \right]_\delta \) was found from MD simulations. The temperature in problems of interest typically varies from \( 0.5 \epsilon / k_B \) to \( 2.0 \epsilon / k_B \), (corresponding to temperatures between \( 60 \text{ K} \) and \( 240 \text{ K} \) for Argon), so \( 0.1 < \delta < 0.2 \). Because in practical situations the temperatures of the wall and the fluid in contact with the wall will be similar, \( \lambda \) will be around 1 according to (6); here \( \lambda \) is sampled from random distribution (11). In this parameter region, one-dimensional MD simulations were performed, solving the equations of motion from Section 2.2, and the remaining coefficient in (15) was fitted as
\[
\left[ \frac{\partial DE}{\partial \lambda} \right]_\delta = -0.682 \epsilon \pm 0.01 \epsilon.
\]

(16)

The result of the fit is shown in Figure 5. Combining the results above, the relation for the exchanged energy during a collision, used in the model, is
\[
DE(\delta, \lambda, \mu) = (1 - \lambda) 0.682 \epsilon.
\]

(17)

Figure 5: Shown in dots is the exchanged energy during the first collision, for several values of \( \delta \) (0.1 < \( \delta < 0.2 \)), between a particle and a vibrating wall for varying \( \lambda \), and \( \mu = 3.6 \) fixed, found from MD simulations. The linear approximation with \( \left[ \frac{\partial DE}{\partial \lambda} \right]_\delta = -0.682 \epsilon \) is shown with a line.
4. RESULTS

4.1 MD simulation with explicit wall

To validate the new boundary condition, it is tested in a situation, where Argon gas is interacting with a hot wall and a cold wall. To simulate Argon molecules with Molecular Dynamics simulations, the Lennard-Jones potential (1) with molecular diameter $\sigma_{Ar} = 0.340 \text{ nm}$, and potential well depth $\varepsilon_{Ar}/k_B = 121 \text{ K}$ is used[13]. Here $k_B$ is Boltzmann’s constant. The mass of an Argon-molecule is $m_{Ar} = 6.6310^{-26} \text{ kg}$. The Calcium wall can be approximated as Lennard-Jones substance with molecular diameter $\sigma_{Ca} = 0.360 \text{ nm}$, mass $m_{Ca} = 6.6510^{-26} \text{ kg}$ and potential well depth $\varepsilon_{Ca}/k_B = 2497 \text{ K}$[18]. When an Argon gas molecule reaches the Calcium wall, the interaction is according to the Lorentz-Berthelot mixing rule[19] by means of a Lennard-Jones potential with $\varepsilon_{Ar-Ca}/k_B = \sqrt{\varepsilon_{Ar}\varepsilon_{Ca}/k_B} = 550 \text{ K}$. The MD simulation uses two walls of 18000 Calcium particles each, with 28154 Argon particles placed in two sections between them. The volume of one gas part is $32 \times 46.9 \times 46.9\sigma_{Ar}^3 = 70387\sigma_{Ar}^3 = 2767 \text{ nm}^3$, and there are 14077 gas particles per section, so the gas density is $n = 0.2m_{Ar}/\sigma_{Ar}^3 = 338 \text{ kg/m}^3$. One Calcium wall is initially 'hot' with temperature $T_h = 240 \text{ K}$, the other wall is initially 'cold' with temperature $T_c = 120 \text{ K}$, and the Argon gas starts with an initial uniform temperature $T_g = 180 \text{ K}$. First, the simulation is allowed to reach an equilibrium, with Berendsen thermostats [20] on both walls so that they keep their temperature. Then, the thermostats are switched off and the temperature development is calculated.

The temperature development of the walls and the gas is shown in Figure 7. It shows that the temperatures of the hot wall and the cold wall converge to $180 \text{ K}$ in several hundred nanoseconds. Note that this example is only meant to examine the heat exchange between gas and wall and is not a realistic simulation of a real micro channel; here only 10 layers of wall molecules are simulated, so the heat capacity is several orders of magnitude lower than in a realistic micro channel.

4.2 MD simulation with new boundary condition

To test the model described in section 2, simulations of particles interacting with a vibrating potential wall were performed, according to the model from Figure 4 and relation (17). The simulation from Section 4.1 was imitated, with the same number of Argon gas particles, but the walls replaced by the new model, shown in Figure 8. Initially, the walls were given temperatures of 120 K and 240 K. With the assumption that all 18000 wall particles have mean energy (kinetic and potential) $3k_B T$, the total wall energy $E_{wall}$ is related to the wall energy $T_w$ according to

$$E_{wall} = 18000 \cdot 3k_B T_w.$$  

After every interaction, the exchanged energy $DE$ was added/removed from this energy reservoir; this assumes that energy is exchanged instantaneously within the wall. After every time step, the new wall temperatures are calculated with (18). The result is shown in Figure 9. Similar to the explicit wall, the temperatures of the hot wall and the cold wall converge to $180 \text{ K}$ in several hundred nanoseconds.
4.3 Explicit walls versus new boundary condition

The results from Section 4.1 and Section 4.2 were derived from the same physical situations. Both models show the temperatures of the hot wall and the cold wall reaching the same value in the same way, as is seen in Figure 10. These similar results were achieved with different simulation times; the explicit wall simulation lasted about 70 hours, while the same simulation with the new boundary condition took about 10 hours.

Although parameter \( \frac{\partial D_E}{\partial t} \delta \), equation (16), was not directly given by the model and had to be fitted from simulations, it was fitted from simulations with a vibrating rigid wall as shown in Figure 2, while the results of the model were compared to an explicit wall simulation as shown in Figure 1. The good agreement of time scale in Figure 10 suggests that models based on a vibrating rigid wall can predict the heat exchange of the more complex explicit wall.

Although the linear relation (17) appears to be a good approximation over a large parameter region, it is not exact, and can differ for certain values of \( \delta \) and \( \lambda \), so the model might not work for special situations outside the scope of this research. Furthermore, the derivation of (17) is based on an ideal gas, and the numerical parameter in (16) has been fitted from a model with only one particle and a wall, whereas in real situations the fluid can be far from ideal, and more particles can simultaneously interact with the wall. Both effects appear to be small, as the results in Section 4 show.
Figure 9: The temperature development in the MD simulation with the new boundary condition based on linear approximation (17), $n = 0.2m_{Ar}/\sigma_{Ar}^3$.

Figure 10: The temperature development in the complete MD simulation compared to the temperature development of the MD simulation with the new boundary condition, $n = 0.2m_{Ar}/\sigma_{Ar}^3$.

5. CONCLUSIONS

For temperatures relevant for Molecular Dynamics simulations, the heat exchange between a fluid and a solid wall was approximated with a linear relation. The linear coefficients were obtained from one-dimensional simulations of an interaction between one particle and a vibrating potential wall. For low temperatures, a fluid particle can have multiple collisions with a wall, but this is ignored in this model. However, our simulations indicated that it can be used in real situations with more simultaneous interactions. As a test, the new boundary condition was compared to an explicit wall in a simulation of a gas between two walls of different temperatures. The heat transfer properties in the two simulations were comparable, but the computation time needed for the implicit boundary condition was small compared to the explicit wall simulation.
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