Dissipative Particle Dynamics (DPD) has, with only a few exceptions, been used to study hydrodynamic behaviour of complex fluids without confinement. Previous studies used a periodic boundary condition, and only bulk behaviour could be studied effectively. However, if solid walls play an important role in the problem to be studied, a no-slip boundary condition in DPD is required. Until now, the methods used to impose a solid wall consisted of a frozen layer of particles. If the wall density is equal to the density of the simulated domain, slip phenomena are observed. To suppress this slip, the density of the wall has to be increased. We introduce a new method, which intrinsically imposes the no-slip boundary condition without the need to artificially increase the density in the wall. The method is tested in both a steady-state and an instationary calculation. If repulsion is applied in frozen particle methods, density distortions are observed. We propose a method to avoid these distortions. Finally, this method is tested against conventional computational fluid dynamics (CFD) calculations for the flow in a lid-driven cavity. Excellent agreement between the two methods is found.
3.1 Introduction

Over the last few years, mesoscopic simulation methods have proven to be a valuable asset in studying the hydrodynamic behaviour of complex fluids. Dissipative Particle Dynamics is one of these methods. Hoogerbrugge and Koelman [1] introduced the method as a way to study suspensions [8]. This coarse grained approach for studying hydrodynamic behaviour could easily be extended to study many other problems involving polymers [10], phase separation [4, 7], and, with the introduction of an energy conserving DPD scheme [17, 16], thermal problems (see Chapter 2).

It is interesting to note that in all simulation studies the simulated system is part of an infinite region. These simulations are performed using standard periodic boundary conditions. To our knowledge, the only exceptions are the work by Kong et al. [14], Jones et al. [30], and Revenga et al. [29]. Kong et al. study the behaviour of a polymer between two walls. The walls are created by freezing the DPD particles so that they can interact with the free particles, while no movement is allowed for these particles. To get an impenetrable wall, the density of the wall is chosen to be four times higher than the confined liquid. It is observed that this high-density wall produces large repulsion near the wall, excluding the solvent and polymer from the wall region. Jones et al. simulate a liquid drop near a solid interface under shear. The solid is again created by freezing the particles at a certain position, either in crystalline or random order. The density of the solid is the same as that of the liquid, but the repulsion between the liquid and the solid is taken higher, producing a strong repulsive layer close to the wall. This causes density distortions in the fluid. Furthermore, the wall created in this way does not impose a no-slip boundary condition for the mean flow. Finally, Revenga et al. create a solid boundary by freezing the particles on the boundary of the solid object. If the density of the constructed wall is equal to that of the fluid, slip at the wall is observed. No-slip can only be approached if the density of the wall is increased. The authors suggest a ratio of nine between the wall and fluid density. In their work no repulsion between
the particles was used, so no low density regions near the wall were obtained. It will be shown that using repulsion within this method will cause strong density distortions near the wall.

Thus, we see that by using a high density layer of frozen particles the no-slip boundary condition can be approached, but it will also change the particle density near the boundary. Now, it depends on the level of coarse graining whether this is a desirable result. On an atomistic level, such a phenomenon is likely to occur near a wall. However, at a higher degree of coarse graining, which we want to pursue in order to study macroscopic flow phenomena, this is an undesirable effect. In this chapter, we will present a method to intrinsically get a no-slip boundary condition without the need for high density walls. Thus, the problem of density distortions near the wall can also be solved.

After briefly introducing the DPD method, the novel boundary condition method is explained. The results of this method are shown for both steady-state shear flow and instationary flow using no repulsion. From these simulations the viscosity is determined. Finally, some methods are explored on how to obtain a flat density profile when using repulsion. These methods are used to calculate the flow inside a lid-driven cavity. The calculated flow field is compared with results obtained with conventional computational fluid dynamics (CFD) calculations.

### 3.2 Dissipative Particle Dynamics

The DPD scheme consists of the calculation of the position and impulses of interacting (fluid) particles over time. The time evolution of these positions \( \mathbf{r}_i(t) \) and impulses \( \mathbf{p}_i(t) \) (for simplicity we take the masses of all particles 1) is given by:

\[
\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i(t), \quad \frac{d\mathbf{v}_i}{dt} = \mathbf{f}_i(t)
\]  

(3.1)

The force acting on the particles is a combination of three parts:

\[
\mathbf{f}_i(t) = \sum_{j \neq i} \left( \mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R \right)
\]  

(3.2)
The first part of the force is the conservative part

\[ F_{ij}^C = \begin{cases} a_{ij} \left( 1 - \frac{r_{ij}}{r_c} \right) \hat{r}_{ij} & (r_{ij} < r_c) \\ 0 & (r_{ij} \geq r_c) \end{cases} \] (3.3)

where \( a_{ij} \) is the maximum repulsion between particle \( i \) and \( j \), \( r_{ij} = r_i - r_j \), \( r_{ij} = |r_{ij}| \), \( \hat{r}_{ij} = r_{ij}/|r_{ij}| \), and \( r_c \) is the cut-off radius. The second and third force are the dissipative and the random force:

\[ F_{ij}^D = -\gamma \omega^D(r_{ij})(\hat{r}_{ij} \cdot \mathbf{v}_{ij})\hat{r}_{ij} \]

\[ F_{ij}^R = \sigma \omega^R(r_{ij}) \theta_{ij} \hat{r}_{ij} \] (3.4)

in which \( \mathbf{v}_{ij} = v_i - v_j \), \( \gamma \) is the friction coefficient and \( \sigma \) is the noise amplitude, \( \omega(r_{ij}) \) is a weight function which tends to zero for \( r = r_c \), and \( \theta_{ij} \) is a random number from a Gaussian distribution with zero mean and \( 1/dt \) variance.

Español and Warren [3] showed that the weight functions and constants in these forces can be chosen arbitrarily, but they should obey:

\[ [\omega^R(r_{ij})]^2 = \omega^D(r_{ij}) \]

\[ \sigma^2 = 2T \gamma \] (3.5)

with \( T \) the temperature of the fluid.

The equations of motion are solved using the modified velocity-Verlet algorithm as presented by Groot and Warren [12]. The weight function for the random force has the following functional form: \( \omega^R(r_{ij}) = 1 - \frac{r}{r_c} \), and we chose \( \sigma = 3.0 \), \( r_c = 1.0 \).

The repulsive interaction is excluded from the simulations unless stated otherwise.

### 3.3 No-slip boundary condition method

A well known boundary condition for imposing (unconfined) simple shear flow, is the Lees-Edwards boundary condition (see for instance [31]), according to which the periodic images at the top and bottom of the simulation box are moving with
a velocity equal to half the box height times the desired shear rate. The boxes at the top and the bottom move in opposite directions. This boundary condition produces a linear velocity profile with the plane of zero velocity in the middle of the simulation box. Notice that in this case the density at the boundary is equal to the density in the simulation box. It is crucial in this boundary condition that the velocity profile continues beyond the boundary of the simulation box, which is not the case when a set of frozen particles is used. In the latter case slip is observed, as noticed in Chapter 2 for thermal problems. In order to explain this slip, one may consider a system that has reached steady-state shear flow. The drag force slowing down a particle is equal to the drag force accelerating it. At a constant density, this is only possible if a linear velocity profile is present everywhere, which is not the case in the boundary where a constant velocity is assigned to the frozen particles. Hence, a steady-state is reached with particles near the boundary having a lower velocity than intended.

In conclusion: to construct a correct no-slip boundary it is necessary to have a velocity profile continuing beyond the boundary. We achieved this not by using a periodic image of the simulation box, but by creating an extra layer of particles, with thickness $r_c$ (the interaction radius) outside the simulation box. The position and velocities of the particles that are in this layer are determined from the position and velocities of the particles within the interaction radius of the boundary. Assume a flow system where a velocity ($V$) in the $y$-direction at $x = 0$ is imposed. For every particle between $x = 0$ and $x = r_c$ a particle is put inside the layer. To easily obtain the desired interpolated velocity profile, the distance to the boundary is kept constant. The tangential velocity of the layer particle is changed in such a way that the mean velocity of the original and the layer particle is equal to the desired boundary velocity ($v_{\text{layer}} = 2 \times V - v_{\text{original}}$), while the normal velocity components get an opposite sign from the original velocity. The $y$ and $z$ positions are given a random shift chosen from the interval $(-r_c,r_c)$. This shift is added since in DPD a particle having a certain $y$ and $z$-velocity has no viscous interaction with another particle having a different $y$ and $z$-velocity, when these particles only differ
in location by their x-position (see Eq. 3.4). Should a DPD particle hit the boundary, a bounce back of this particle is induced.

Simulations have been performed with this new boundary condition method in an $8 \times 8 \times 8$ sized simulation box, containing 12800 ($\rho = 25$), 8960 ($\rho = 17.5$), and 5120 ($\rho = 10$) particles. The time step is chosen such that $\gamma \delta t = 5 \cdot 10^{-2}$, and the imposed velocity is 0.5 at $x = 0$ and 0.0 at $x = 8$. In Figure 3.1 the averaged (over $10^4$ timesteps) stationary velocity profile is plotted. The agreement with the theoretical solution is excellent.

Figure 3.1: Average $y$-velocity of the particles in the 16 bins dividing the x-axis. Three temperatures ($T = 0.01, 0.1$ and $1.0$) and three number densities ($\rho = 10, 17.5$ and 25) are shown, together with the theoretical solution.
3.4 Determining the kinematic viscosity

As a further test of our new implementation of the no-slip boundary condition, we chose the following classical example: suppose a fluid occupying the space from $x = 0$ to $x = \infty$ is initially at rest. At time $t = 0$, the velocity at $x = 0$ is raised to $v_1$ and kept at this value. A velocity profile will develop according to:

$$\frac{\partial v}{\partial t} = v \frac{\partial^2 v}{\partial x^2}$$

(3.6)

with $\nu$ the dynamic viscosity of the fluid. The solution of this problem is known to be [28]:

$$\frac{v}{v_1} = 1 - \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{4\nu t}} \exp^{-\eta^2} \, d\eta = 1 - \text{erf} \left( \frac{x}{\sqrt{4\nu t}} \right) = \text{erfc} \left( \frac{x}{\sqrt{4\nu t}} \right)$$

(3.7)

The dynamic viscosity can now be found readily from a DPD simulation by fitting this formula onto a simulated velocity profile at a certain time. Simulations shown here are from the $\rho = 25$ calculations at $T = 0.1$. Results from such a fit are shown in Figure 3.2. The dynamic viscosity is estimated from the first simulation time and used to predict the other two simulation results. The agreement between prediction and simulation is very good, and the boundary condition is satisfied throughout the whole simulation, showing that accurate, instationary confined fluid simulations using DPD are possible.

As an alternative to determining the viscosity from instationary profiles, it can be computed from stationary shear flow. The shear stress can be determined (see for instance [31]) using:

$$\tau_{xy} = \frac{1}{V} \sum_{i<j} F_{y,ij} r_{x,i} + \frac{m}{V} \sum_i (v_{x,i} - v^*_x) \cdot (v_{y,i} - v^*_y)$$

(3.8)

in which $V$ is the volume of the system, $m$ is the particle mass, $F_{y,ij}$ is the $y$-component of the force exerted on particle $i$ by particle $j$, $r_{x,i}$ is the $x$-position of particle $i$, $v_{y,i}$ and $v_{x,i}$ are the $y$ and $x$ components of the velocity respectively, and $v^*$ is the theoretical value of the velocity.
Figure 3.2: Average $y$-velocity of the particles in the 16 bins dividing the $x$-axis. The symbols represent the simulation results and the lines give the prediction based on the fit on the first temperature profile. Three simulation times ($t = 0.1, 0.4$ and $0.9$) are plotted.

Figure 3.3: Kinematic viscosity as determined with the conventional steady-state calculation and the instationary method.
The shear stress has been obtained by averaging over some $10^5$ timesteps. Results of these calculations are given in Figure 3.3 together with the results from the instationary calculations. Both methods yield the same results, although the instationary calculations are computationally less expensive. The line in the graph represents the kinetic theory result by Marsh et al. [25] ($\nu = \frac{\pi \rho_0^2}{1575T}$) for the dissipative contribution only. Viscosities calculated by us are somewhat lower, but such a discrepancy between calculated viscosities and this theoretic prediction has been noticed before [32, 33].

3.5 Density profiles for different boundary conditions

Another incentive for our implementation of the no-slip boundary condition is to achieve a flat density profile throughout the simulation box, even though a boundary is present. However, when a repulsive force was added to our calculations ($\alpha_{ij} = 25$), a certain effect of the boundary on the density profile was observed. To explore this behaviour, we made a plot of the conservative force exerted by the boundary onto the fluid. Simulations have been performed in a $15 \times 8 \times 8$ sized box containing 9600 particles ($\rho = 10$) at $T = 1.0$. In the case of our boundary condition method, which means creating an extra layer of particles beyond the boundary, the repulsive force close to the boundary is too high. This causes a decrease of the density in this region, as can be seen from Figure 3.4. For this reason, some attempts have been made to implement the repulsive force in a different way, while applying the original calculation method for the dissipative and random force, since this yields a very good treatment of the no-slip boundary condition.
Figure 3.4: Density profile as calculated with the various implementations of the repulsive force of the boundary; the original mirrored way, a uniformly distributed, a single layer of particles, and the shifted particle method.

Figure 3.5: Resulting repulsive wall force as calculated with the various positioning of the boundary particles; the original mirrored way, a uniformly distributed, a single layer of particles, and the shifted particle method.
If we would assume a uniform density in the extra layer, the repulsive force of this layer can be solved analytically. This leads to $F^C_x = a_{ij} \frac{r_0}{12} (1 - x)^3 (1 + 3x)$. However, again some small distortions in the density profile were observed. This is due to the fact that the analytical solution does not assume a spatial correlation between the particles. In an attempt to preserve spatial correlation, the interaction with the layer particles is split into two parts. First, we create a layer of particles as described above (see section 3.3), from which the drag and random forces are calculated. Then, a second set of layer particles is created, from which the repulsive interaction is calculated. The positions of the particles in the second set are determined by shifting all the particles located at a distance between $r_c$ and $2r_c$ from the boundary into this layer. A spatial correlation should exist between the particles next to the wall and the ones between $r_c$ and $2r_c$. In Figure 3.4 the results from these calculations are given, showing that this method leads to an almost flat density profile. For the sake of comparison, also the density profile and wall force are determined for the case of one layer of particles located exactly at the boundary (as used in [29]). Clearly, the wall force (see Figure 3.5) is completely different in shape, leading to an undesirable density profile. In this case, the region near the boundary is completely depleted of particles.

### 3.6 Testcase: lid-driven cavity

In order to validate the method proposed above to treat the repulsive particle interactions, the flow inside a lid-driven cavity has been calculated. A lid-driven cavity consists of a two-dimensional box, of which the lid is moving with a certain velocity. The flow inside such a geometry has been studied extensively both experimentally [34] and computationally [35]. Here, a comparison is made between the results from the DPD method and the commercial Computational Fluid Dynamics (CFD) package Fluent.
The 3D DPD calculation has been performed in a $10 \times 10 \times 4$ sized box containing 4000 particles ($\rho = 10$) at $T = 0.33$. The repulsion parameter $a_{ij}$ is 3.0 and the viscosity of this fluid was determined to be 0.517. The lid is moving with a speed of 0.517 leading to a Reynolds number of 10. The velocity is determined by averaging in space over a $x, y$-grid of $32 \times 32$, and in time over $10^6$ timesteps. These calculations took 36 hours on a Pentium-II 400 machine. The 2D CFD calculations have been performed on a $128 \times 128$ grid with dimensions $1.0 \times 1.0$ a viscosity of 0.1, and a velocity of 1.0, again leading to a Reynolds number of 10. These calculations took 4 hours on the above mentioned machine, to achieve a residual of $5 \cdot 10^{-4}$ for all variables.

Results of DPD and CFD computations are depicted in Figures 3.6 and 3.7. In the first figure the flow field is shown. The agreement between the two methods is very good, only in the top left and right corners small differences can be observed. This is due to the fact that in the corner the velocity is not well defined, since, in principle, it should obey the boundary condition of both walls, which leads to an inconsistency. The two methods treat this inconsistency in different ways, which explains the different velocities near the corners.

The second figure shows the $x$ and $y$ velocity at the centreline of the cavity. The agreement between the two methods is excellent. The only difference between the two methods is the simulation time. Note, however, that the CFD calculations were performed in two dimensions only. Evidently, this demonstrates that DPD and CFD yield identical results for flow systems. However, it should be realised that the great potential of DPD is not present in classical flow problems, but in problems where the continuum approach of CFD fails. Typical examples are multiphase flow and polymeric liquids with complex rheology (viscoelasticity).
3.6 Testcase: Lid-driven cavity

Figure 3.6: Comparison of the flow field as calculated with a commercial CFD package (Fluent) and with the DPD method.

Figure 3.7: Comparison of the $v_x$ and $v_y$ at $x = 0.5$ and $y = 0.5$ as calculated with the CFD package (Fluent) and the DPD method.
3.7 Concluding remarks

In this chapter, we have introduced a novel implementation of a no-slip boundary condition within the dissipative particle dynamics simulation method. This method intrinsically imposes a no-slip boundary condition. Care must be taken when repulsive interactions between the particles come into play. This will require a special positioning of the boundary particles for which the spatial correlation within the fluid is preserved. Shifting the particles located at a distance between $r_c$ and $2r_c$ from the boundary meets this requirement, as can be seen from the results for flow inside a lid-driven cavity.