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Backer, J.A.; Lowe, C.P.; Hoefsloot, H.C.J.; Iedema, P.D.

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# Poiseuille flow to measure the viscosity of particle model fluids

J. A. Backer,[a] C. P. Lowe, H. C. J. Hoefsloot, and P. D. Iedema
*Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Nieuwe Achtergracht 166,*
*1018 WV Amsterdam, The Netherlands*

The most important property of a fluid is its viscosity, it determines the flow properties. If one simulates a fluid using a particle model, calculating the viscosity accurately is difficult because it is a collective property. In this article we describe a new method that has a better signal to noise ratio than existing methods. It is based on using periodic boundary conditions to simulate counter-flowing Poiseuille flows without the use of explicit boundaries. The viscosity is then related to the mean flow velocity of the two flows. We apply the method to two quite different systems. First, a simple generic fluid model, dissipative particle dynamics, for which accurate values of the viscosity are needed to characterize the model fluid. Second, the more realistic Lennard-Jones fluid. In both cases the values we calculated are consistent with previous work but, for a given simulation time, they are more accurate than those obtained with other methods. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1883163]

## I. INTRODUCTION

The viscosity of a fluid is the main parameter that determines its flow characteristics. Realistic fluids, for which the rheological behavior is of intrinsic interest, can be simulated with particle models, notably molecular dynamics (MD).[1] Recently, the idea of using simpler particle models, intended to reproduce hydrodynamic behavior, has also been applied in an attempt to overcome the time scale limitations inherent in molecular dynamics.[2–4] In these simple model fluids the viscosity generally has to be measured because sufficiently accurate theoretical expressions are lacking.[5] That is, ideally the viscosity would be an input parameter but in practice the simulation must be "calibrated". There are several methods available to calculate viscosity, all with their relative advantages and disadvantages. In this article we describe a novel method that we show is advantageous in some circumstances. We begin with a review of the techniques currently available.

A division can be made between equilibrium and nonequilibrium methods. In the first the simulated system is first equilibrated and subsequently remains in equilibrium. The viscosity is then calculated from the stress–stress autocorrelation function through the Green–Kubo relation.[1] Because the system is in equilibrium, simple periodic boundary conditions are adequate. Furthermore, the shear rate is by definition zero, so one is automatically in the linear regime. These facts make this method very appealing, but unfortunately the large fluctuations in the equilibrium stress lead to a poor signal to noise ratio. An alternative equilibrium method, proposed by Palmer,[6] is based on the transverse-current autocorrelation function. One can extract the viscosity from the decay of this function, if one assumes the hydrodynamic prediction for its functional form. This additional assumption means that it is not obviously prefer-

able to the stress–stress autocorrelation function, although it is efficient for purely dissipative systems.[7] Hess has compared these two equilibrium methods to nonequilibrium methods in molecular-dynamics simulations.[8] His results show that, despite their undoubted advantages, both equilibrium methods suffer from worse statistics than nonequilibrium methods.

In nonequilibrium methods the fluid is subjected to an external perturbation that may be constant or temporally varying. The properties of the nonequilibrium steady state or the decay to the equilibrated state are then related to the viscosity. One example is a periodic perturbation employed to generate an oscillatory velocity profile,[9] depending on the frequency of the sinusoidal external force. Several measurements at different frequencies and extrapolation to zero-frequency are required to determine the viscosity. A more recent method[10] imposes a pulsed Gaussian velocity profile on the system. The decay of the Gaussian peak gives an estimate of the viscosity. Müller-Plathe obtains a linear velocity profile by cleverly swapping impulses of spatially remote particles.[11] The interchanged momentum and the measured velocities provide the viscosity. More common is the converse procedure, imposing a linear profile at a fixed shear rate and measuring the resultant shear stress. This shear flow method is the underlying principle of most experimental rheometers. In simulations, however, problems arise at the boundaries of the simulation domain, as periodic boundary conditions are not able to maintain a steady linear velocity profile. Ways around this include stochastic boundary conditions[12] and Lees–Edwards boundary conditions.[13] The latter retain periodicity but alter the position and velocity of the periodic images. An important advantage of the shear flow method is the constant shear rate, which enables one to study the dependence of the viscosity on the shear rate. For example, the viscosity of a dissipative particle dynamics (DPD) model of a colloidal suspension was studied using this approach.[14] The shear flow method is also successfully

a)Electronic mail: backer@science.uva.nl

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applied to determine the viscosity in stochastic rotational dynamics (SRD) models.[15] Less widely used is a similar "flow" method that uses a Poiseuille flow profile. The problem with this approach is that the boundary condition issues are still unresolved. Considerable density fluctuations near the system boundaries are present in MD simulations,[16] SRD simulations[17] as well as DPD simulations.[18] Relative to equilibrium methods extra care is needed when using any non-equilibrium method. The use of external fields causes viscous heating. The energy supplied to the system causes the temperature to rise monotonically for a steady perturbation. In that case a heat sink is required to drain the excess energy, e.g., through the use of a thermostat. Furthermore, the flow needs to be in the linear regime and extrapolation to the zero perturbation limit may be required.

Concluding from the existing literature, the stress autocorrelation method and the shear flow method are favored in most particle models to measure the viscosity. In this paper we propose an improvement of the Poiseuille flow method by introducing periodicity, that solves the boundary problem. We compare the new method to the stress autocorrelation and shear flow method and show its advantages, both in accuracy of the results and in ease of implementation. For the comparison of the methods, DPD simulations are a useful tool. Viscous heating is absent because of the built-in thermostat, and DPD fluids exhibit Newtonian behavior over a large range of parameters.[3] The periodic Poiseuille flow method is not limited to DPD but can also be applied in other particle models. To illustrate this, we use the same methodology to calculate the viscosity of a Lennard-Jones fluid in an MD simulation. The rest of this paper is organized as follows. Section II proposes a periodic Poiseuille flow method. The computational details of the DPD and MD simulations are given in Sec. III. Section IV first presents and discusses the results of the new method. Then a comparison between different techniques at different parameter sets is made. The section concludes with the results for the MD simulations. In Sec. V we draw conclusions from the present work.

## II. PERIODIC POISEUILLE FLOW METHOD

Poiseuille flow is obtained by applying a body force, such as a gravitational force or pressure gradient, to each particle. For instance, if gravity works in the $z$ direction on a fluid between two plates in the $xy$-plane, the resulting flow field has a linear shear stress profile and a parabolic velocity profile[19]

$$\tau_{xz} = \rho g_z(x - \tfrac{1}{2}D), \tag{1}$$

$$v_z = \frac{\rho g_z}{2\eta}(xD - x^2). \tag{2}$$

In these equations $\tau_{xz}$ is the shear stress, $v_z$ is the velocity directed parallel to the force, $\eta$ is the dynamic viscosity, $\rho$ is the mass density, $g_z$ is the gravitational constant, $x$ is the position between the two plates, and $D$ is the distance be-
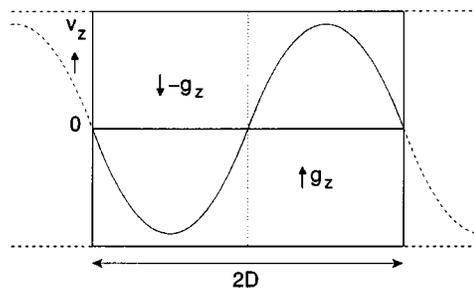


FIG. 1. Schematic representation of the periodic Poiseuille flow method.

tween the plates. Integration of Eq. (2) with respect to $x$ over the distance between the plates $D$ gives the system average of the velocity $\langle v_z \rangle$

$$\langle v_z \rangle = \frac{1}{D}\int_0^D v_z(x)dx = \frac{\rho g_z D^2}{12\eta}. \tag{3}$$

Measurement of this system average directly gives the viscosity of the fluid. Note that this derivation assumes a constant density in the simulation domain and a constant viscosity over varying shear rates. The shear rate $dv_z/dx$ ranges from zero, where the velocity is at a maximum, to a maximum value where the velocity is zero. So, in contrast to the shear flow method, this method is not suitable for determining the shear rate dependent viscosity. It is limited to fluids in the Newtonian regime.

Periodic boundary conditions are not sufficient, because they cannot keep the fluid at zero velocity at the edges of the simulation domain. To circumvent this problem Kauzlarić *et al.* implement stochastic boundary conditions[18] and Allahyarov and Gompper use a bounce back condition.[17] However, in both cases the density profile shows artefacts at the boundary. An easier solution to this problem is to subdivide the system into two domains, and apply a body force in the opposite direction in the two domains. Figure 1 explains this idea schematically. Because of the periodic boundary conditions the counteracting body forces constrain the fluid at the positions where the plates would be. Note that to obtain the system average, the velocity $v_z$ has to be measured in the direction of the external force.

Summarizing, the proposed Poiseuille flow method is limited to fluids in the linear regime. Despite this drawback it could have significant advantages over other methods. We expect a more accurate result compared to the shear flow method, as the system average of the velocity is less susceptible to noise than the shear stress average. This is because, in continuum terms, the shear stress is related to a derivative of the velocity field. The body forces are easily implemented, and when opposing forces are applied, ordinary periodic boundary conditions can support the parabolic flow fields.

## III. COMPUTATIONAL DETAILS

Three different viscosity measurement techniques, the stress autocorrelation method, the shear flow method and the periodic Poiseuille flow method, are compared in simulations. We use dissipative particle dynamics (DPD), a mesoscale particle model that was introduced by Hoogerbrugge

and Koelman[3] in 1992 and put on a sounder theoretical footing by Español and Warren.[20] In short, every particle is meant to represent a fluid element that experiences other fluid elements within a relatively small cut-off radius $r_c$. They are kept in motion by a random force and counteracted by a drag force depending on the velocity of surrounding particles. Together these counteracting forces act as a thermostat. All forces are finite and smooth allowing for large time steps. For details on the algorithm we refer the reader to Groot and Warren.[21] For our purposes DPD has many advantages over other particle methods. Because of the small cut-off radius $r_c$, the stress autocorrelation function does not suffer from finite size effects. The thermostat removes the risk of viscous heating and, due to the large time step, simulations do not take much computation time. Conservative forces are not needed for this study and will be left out.

Marsh et al. derived an estimate for the dynamic viscosity $\eta$ based on kinetic theory.[5] There are two contributions to the viscosity. The first term is a kinetic contribution originating from the motion of the individual particles and the second term is a dissipative contribution from the energy dissipation between particles

$$\eta = \frac{45}{2\pi}\frac{(k_B T)^2}{\sigma^2 r_c^3} + \frac{\pi}{1575}\frac{n^2\sigma^2 r_c^5}{k_B T}. \qquad (4)$$

Here $n$ is the number density, $\sigma$ the noise amplitude that drives the random force, $T$ the temperature, and $k_B$ Boltzmann's constant. Although the trends are well described by Eq. (4), the prediction deviates considerably from the actual viscosity. It can, however, help in the parameter choice. The viscosity of a liquid is mainly attributed to the dissipative term, whereas viscosity of a gas is largely determined by the kinetic contribution. As we are interested in measurements in the liquid regime, we should choose the parameters accordingly. Equation (4) shows that a large noise amplitude $\sigma$, low temperature $k_B T$, and a high number density $n$ achieve this objective. We choose the parameters for the base case as noise amplitude $\sigma=4.5$, number density $n=6$ and temperature $k_B T=0.5$, in units where the particle mass and the cut-off radius $r_c$ are unity. Furthermore, the time step $\Delta t=0.01$ and the simulation box size is $12\,r_c$ in $x$ direction and $8\,r_c$ in $y$ and $z$ direction. The simulation time after equilibration is 100 time units, but when calculating profiles for the periodic Poiseuille flow method one long run of 1000 time units is performed. For the comparison of the viscosity measurement methods the noise amplitude, number density, and temperature are varied. We repeat the simulation for each parameter set for each measurement method 10 times, from which the average viscosity and standard deviation are calculated.

For the stress autocorrelation function the shear stress in three directions is calculated at every time step. The maximum correlation time is set to 20 and the viscosity is calculated from the average over the last half of the integrated correlation function, where the stress–stress autocorrelation function is statistically indistinguishable from zero. The linear velocity profile required in the shear flow method is achieved with Lees–Edwards boundary conditions.[13] For the shear flow method as well as the Poiseuille flow method the external force must be determined. For each parameter set a

test run is performed to get an estimate for the viscosity. Based on this preliminary viscosity and the requirement for a small Reynolds number ($Re=\rho\langle v_z\rangle D/\eta$, here we take Re $=4$) the average velocity in the flow direction is calculated. For the shear flow method the shear velocity is twice this average velocity. The corresponding body force for the Poiseuille flow method is calculated from Eq. (3). For both flow methods the estimated velocity profile is imposed on the particles at the start of the simulation. Measurements take place every 10 time steps and the velocities are corrected by the addition of a constant factor every 100 time steps to enforce the condition of zero total momentum.

The three methods are also used to measure the viscosity of a Lennard-Jones fluid with molecular dynamics at constant NVT.[1,22] In contrast to the DPD simulations, only one state point is considered, at a reduced[1] number density $n=0.8442$ and reduced temperature $T=0.722$. The cut-off radius for the Lennard-Jones potential is $r_c=2.5$ and the time step is $\Delta t=0.001$. Because two of the methods involve an external force, a thermostat is required to keep the temperature constant. The DPD thermostat (i.e., the random and dissipative forces) can be used for this purpose,[23] but we choose the Lowe–Andersen thermostat[24] instead. This avoids any time step dependence of the temperature. The collision parameter is $\Gamma=20$ and the cut-off radius for the thermostat is $r_c^{th}=1.1$. As this thermostat enhances viscosity, the system in equilibrium for the stress autocorrelation method must also be thermostatted. In this way we can compare the results of the three methods. For the stress autocorrelation method the average of the Green–Kubo integral from 10 to 30 time units is taken to determine the viscosity. For the shear flow method the shear velocity is $V_{shear}=0.04$ and for the periodic Poiseuille flow method the body force is $g_z=0.02$. These external forces result in a maximum velocity well below the kinetic velocities. The simulation domain is a relatively large cube of volume $16^3$. The simulations are run for 200 time units after an equilibration time of 50 time units and repeated ten times.

## IV. SIMULATION RESULTS AND DISCUSSION

In this section we first examine the DPD results of the periodic Poiseuille flow method for the base case. Next, we compare the DPD results of the stress autocorrelation method, the shear flow method and the periodic Poiseuille flow method over a range of parameters. Finally, we compare the three methods for determining the viscosity of a Lennard-Jones fluid at one state point.

### A. Results of the periodic Poiseuille flow method

A long simulation for the base case parameters ($n=6$, $\sigma=4.5$, and $k_B T=0.5$) and an external force of $g_z=0.055$ allows us to determine the profiles of various properties to assess the periodic Poiseuille flow method in detail. The density profile, shown in Fig. 2, is uniform except for statistical fluctuations. Density artefacts as found in other implementations of the Poiseuille flow[17,18] are absent in our method, as is required for a bulk Poiseuille flow.
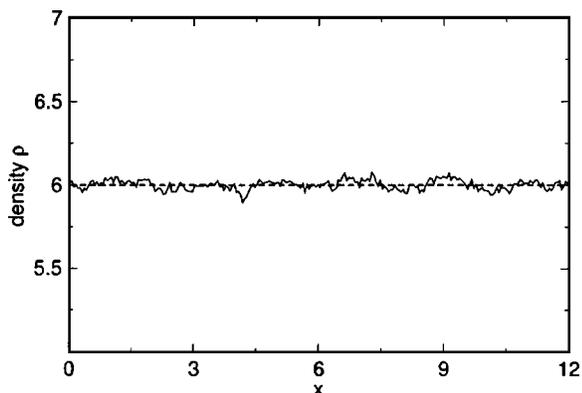
FIG. 2. Density profile for periodic Poiseuille flow method: Measured profile (solid line) and theoretical value (dashed line).



FIG. 4. Velocity profile for periodic Poiseuille flow method: Measured profile (solid line) and theoretical value (dashed line).

The difference between the particle velocities and the local velocity based on the instantaneous viscosity is measured to plot the temperature profile. The measured temperature was 2% lower than the input value, because the time step of $\Delta t = 0.01$ proved to be too large for the thermostat to work properly. This is a well known artefact of the simple DPD algorithm,[5,25] which is resolved in the Lowe–Andersen thermostat.[24] To distinguish between the effect of a large time step and viscous heating, the same simulation was performed with a smaller time step of $\Delta t = 0.001$. The resulting temperature profile is shown in Fig. 3. Although the shape of a parabolic profile is present, the deviations from the input value are sufficiently small to neglect viscous heating.

The measured velocity profile is shown in Fig. 4 together with the parabolic flow field [Eq. (2)] based on the measured viscosity. To within an accuracy of 0.1% the profile agrees with the analytic laminar Poiseuille flow field. This justifies the use of the average velocity as a means to calculate the viscosity [Eq. (3)].

The shear stress is determined from the pair interactions and particle velocities.[1] In Fig. 5 we show that the shear stress profile is linear in accordance with Eq. (1), and shows a sudden change at the extreme values due to the switch of the direction of the external force. The deviations from the theoretical stress profile are not statistically significant.

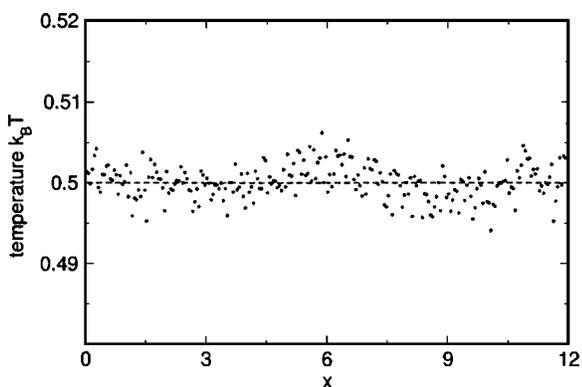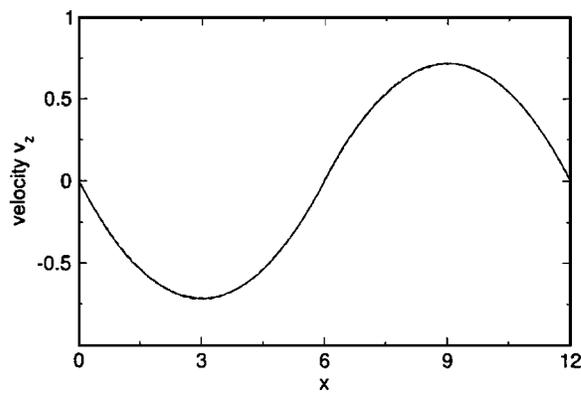The measured viscosity is $\eta = 2.09 \pm 0.02$, based on the overall average of the velocity. To test whether this viscosity is constant over all shear rates, i.e., whether the liquid is in the Newtonian regime, we determine the viscosity as a function of the shear rate. From the velocity profile the local velocity gradient at each position is computed from the velocities of the two neighboring data points. As the slope of the parabolic profile is a linear function of the position, this procedure should be sufficiently accurate. For a Newtonian fluid the ratio of the measured shear stress and the local velocity gradient gives the local viscosity. This is plotted against the local shear rate in Fig. 6. The viscosity is equal to the measured overall viscosity for high and intermediate shear rates. The scatter at low shear rates reflects the larger numerical errors due to the small values for both the shear stress and the velocity gradient. This results in a large error in their ratio. Given this, we find no evidence that the fluid is not Newtonian. It should be emphasized again that this is not a way to measure shear rate dependent viscosities. If the viscosity is not constant, the measured average velocity will in fact reflect the effects of the spatially varying viscosity.

## B. Comparison of viscosity measurement techniques in DPD

We calculate the viscosities for different parameter sets with the three different methods. Figure 7 shows the viscosity with error bars as a function of density. The measured averages of the three methods agree well within their error bars, but the size of the error bars differs greatly. As ex-



FIG. 3. Temperature profile for periodic Poiseuille flow method: Measurements (solid dots) and theoretical value (dashed line).
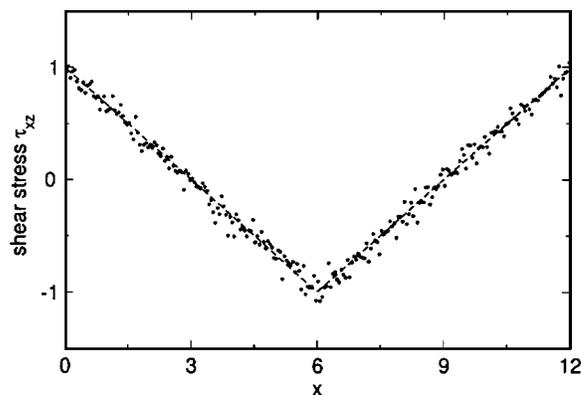


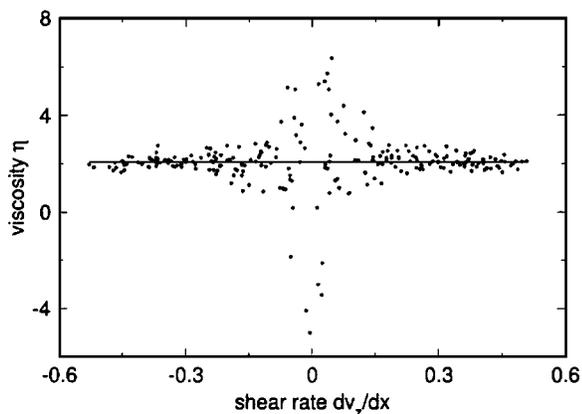FIG. 5. Shear stress profile for periodic Poiseuille flow method: Measurements (solid dots) and theoretical value (dashed line).

FIG. 6. Viscosity as a function of shear rate: Measurements (solid dots) and value based on the average velocity measurement (solid line).



FIG. 8. Viscosity as a function of noise amplitude, measured with stress autocorrelation function ($\bigcirc$), shear flow method ($\square$) and periodic Poiseuille flow method ($\triangle$); symbols are horizontally shifted for clarity purposes.

pected, the stress autocorrelation method is the least accurate. Of the two flow methods the periodic Poiseuille flow method gives the better results. The error bars of these two methods do not change significantly over the density range, because the simulations are performed at similar Reynolds numbers.

The viscosity as a function of noise amplitude, plotted in Fig. 8, also shows that the averages from all methods are in agreement. Again the error bars of the shear flow method are smaller than for the autocorrelation method, but larger than for the Poiseuille flow method. The accuracy of the stress autocorrelation method deteriorates with increasing noise amplitude. This is because the dissipation in the system increases and the fluctuation in the stress measurements is mainly due to the dissipative part. This effect is not apparent for the shear flow method, as the collective motion dominates the chaotic motion of the particles. The error bars do not change due to the constant Reynolds number. For the periodic Poiseuille flow method the standard error shows no discernible trend.

The measured viscosities at different temperatures in Fig. 9 agree within the statistical accuracy for the three methods. The stress autocorrelation method gives poor results at low temperatures, but gains in accuracy with increasing temperature. The cause is the smaller role of the dissipation in
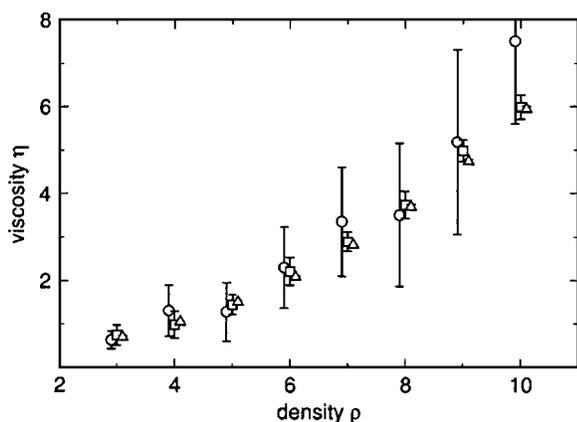
the stress measurements, as explained above. Again, the error bars of the flow methods are not affected by the change in temperature. The most accurate over all temperatures is the periodic Poiseuille flow method.

A comparison between the methods is made, based on the average accuracy of all parameter sets. We estimate that the periodic Poiseuille flow method is 10 times as accurate as the shear flow method and 30 times as accurate as the stress autocorrelation method. Of course these ratios depend on the parameter set and are only mentioned to illustrate the disparate relative performance. A more significant measure to compare the methods is the number of measurements needed to arrive at a result within a certain confidence interval. To this end we performed 100 independent simulations with the base case parameters for each measurement method. The 100 viscosity results are grouped in sets of $N$ measurements, where $N$ ranges from one to ten. The average deviation of the sets from the overall average is plotted in Fig. 10 as a function of set size $N$. The figure shows that a single measurement of the autocorrelation method can deviate 30% from the actual viscosity, i.e., the average of 100 measurements. Even ten measurements lead to an average that is unacceptably inaccurate. The shear flow method does achieve acceptable results but requires multiple measurements, while for the periodic Poi-
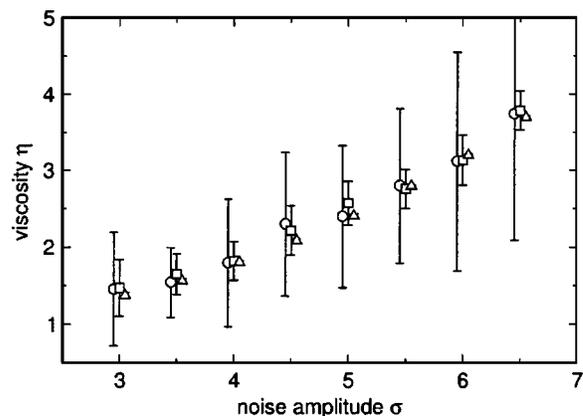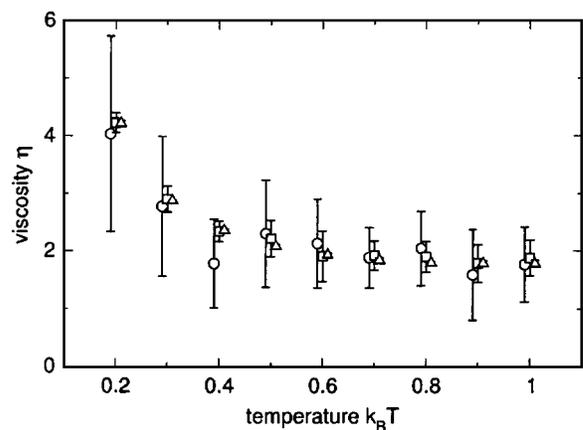


FIG. 7. Viscosity as a function of density, measured with stress autocorrelation function ($\bigcirc$), shear flow method ($\square$) and periodic Poiseuille flow method ($\triangle$); symbols are horizontally shifted for clarity purposes.



FIG. 9. Viscosity as a function of temperature, measured with stress autocorrelation function ($\bigcirc$), shear flow method ($\square$) and periodic Poiseuille flow method ($\triangle$); symbols are horizontally shifted for clarity purposes.
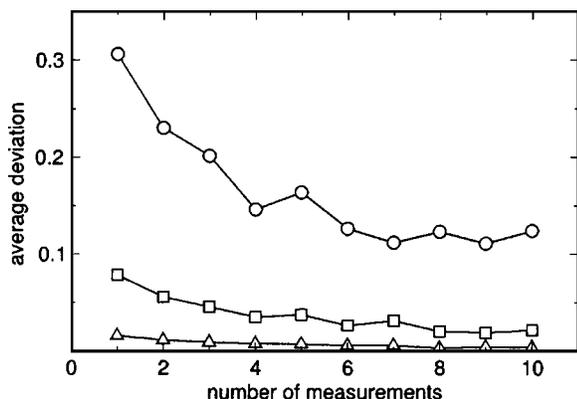
FIG. 10. Average deviation of viscosity from average viscosity as a function of number of measurements for stress autocorrelation method (-○-), shear flow method (-□-) and periodic Poiseuille flow method (-△-).

seuille flow method all single measurements are within a 98% confidence interval. Thus, even one short simulation is sufficient to achieve accurate results.

## C. Comparison of viscosity measurement techniques for a Lennard-Jones fluid

Finally, we test the three methods on a Lennard-Jones fluid at a reduced density of $n=0.8442$ and reduced temperature of $T=0.722$. At this state point, Meier *et al.* collected the results of several studies.[26] They report viscosities ranging from 2.7 to 4.0, depending on measurement technique, simulation time and system size. Our results are as follows:

(i)      Stress autocorrelation method: $\eta=3.7\pm1.2$;
(ii)     shear flow method: $\eta=3.4\pm0.8$;
(iii)    periodic Poiseuille flow method: $\eta=3.4\pm0.2$,

well within the range quoted in Ref. 26. The average viscosities of the three methods are in agreement. As expected the stress autocorrelation method gives the least accurate results, while the periodic Poiseuille flow method is four times as accurate as the shear flow method. This example illustrates that the periodic Poiseuille flow method is not only limited to simple fluid models, but is applicable to realistic systems as well. The latter often involve long simulation times, that can be reduced considerably by our more accurate method. We should point out though, that the nonuniform shear stress means the method is restricted to the Newtonian regime.

## V. CONCLUSION

The Poiseuille flow method to measure the viscosity in a particle model is improved, guaranteeing a flat density pro-file throughout the simulation domain. Shear stress measurements are not required, as the system average of the velocity in the flow direction directly provides the viscosity of the fluid. Moreover, the application of opposing external forces enables the use of ordinary periodic boundary conditions.

Series of DPD simulations were performed to measure the viscosity with the stress autocorrelation method, the shear flow method and the periodic Poiseuille flow method. The methods give comparable results for the average of the measured viscosity, but the accuracy differs greatly. Being an equilibrium method, the stress autocorrelation method is the least accurate. The periodic Poiseuille flow method gives the best results, roughly ten times as accurate as the shear flow method. Also for a Lennard-Jones fluid our method proves to be advantageous. Thus, the periodic Poiseuille flow method reduces the computation time needed to determine the viscosity of a particle model fluid.

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