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## **Molecular Dynamics Simulations of Microscale Fluid Transport**

C. C. Wong, A. R. Lopez, M. J. Stevens, S. J. Plimpton

Prepared by

Sandia National Laboratories

Albuquerque, New Mexico 87185 and Livermore, California 94550

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## **Molecular Dynamics Simulations of Microscale Fluid Transport**

C. C. Wong, A. R. Lopez, M. J. Stevens, S. J. Plimpton  
Engineering Sciences Center  
Computational Sciences, Computer Sciences, & Mathematics Center  
Sandia National Laboratories  
P. O. Box 5800  
Albuquerque, NM 87185-0827

### **Abstract**

Recent advances in micro-science and technology, like Micro-Electro-Mechanical Systems (MEMS), have generated a group of unique liquid flow problems that involve characteristic length scales of a micron. Also, in manufacturing processes such as coatings, current continuum models are unable to predict microscale physical phenomena that appear in these non-equilibrium systems. It is suspected that in these systems, molecular-level processes can control the interfacial energy and viscoelastic properties at the liquid/solid boundary.

A massively parallel molecular dynamics (MD) code has been developed to better understand microscale transport mechanisms, fluid-structure interactions, and scale effects in micro-domains. Specifically, this MD code has been used to analyze liquid channel flow problems for a variety of channel widths, e.g. 0.005-0.05 microns. This report presents results from MD simulations of Poiseuille flow and Couette flow problems and address both scaling and modeling issues. For Poiseuille flow, the numerical predictions are compared with existing data to investigate the variation of the friction factor with channel width. For Couette flow, the numerical predictions are used to determine the degree of slip at the liquid/solid boundary.

# Acknowledgment

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## Summary

Recent advances in micro-science and technology, like Micro-ElectroMechanical Systems (MEMS), have generated a group of unique liquid flow problems that involve characteristic length scales of a micron. Traditional approaches are unable to analyze microscale transport phenomena. This problem may be due to the continuum or equilibrium assumption breaking down for liquid flows in microscale geometries or under high stress. Also, in manufacturing processes such as coatings, current continuum models are unable to predict wetting/de-wetting phenomena for non-equilibrium systems. It is suspected that in these systems, molecular-level processes can control the interfacial energy and viscoelastic properties at the liquid/solid boundary.

A massively parallel molecular dynamics (MD) code has been developed to address this new class of non-equilibrium, transport problems for microscale structures. The new capability will help better understand microscale transport mechanisms, fluid-structure interactions, and scale effects in micro-domains. Specifically, this MD code has been used to analyze liquid channel flow problems for a variety of channel widths, e.g. 0.005-0.05 microns. This report presents results from MD simulations of Poiseuille flow and Couette flow problems and address both scaling and modeling issues. For Poiseuille flow, the numerical predictions are compared with experimental data to investigate the variation of the friction factor with channel width. For Couette flow, the numerical predictions are used to determine the degree of slip at the liquid/solid boundary. Finally, our results also indicate that shear direction with respect to the wall lattice orientation can be very important. Simulation results of microscale Couette flow and microscale Poiseuille flow for two different surface structures and two different shear directions will be presented.



# Molecular Dynamics Simulations of Microscale Fluid Transport

## 1. Introduction

Recent advances in micro-science and technology, like in MicroElectroMechanical Systems (MEMS), in the fabrication of metal/ceramic composites, and also in bio-engineering, have generated a group of unique fluid flow problems that involve characteristic length scales of a micron. Traditional continuum and equilibrium approaches are unable to analyze these microscale transport phenomena. This problem may be due to the continuum or equilibrium assumption breaking down for fluid flows in microscale geometries or under high stress. For example, MEMS researchers at the University of California, Los Angeles<sup>1</sup> and University of Pennsylvania<sup>2</sup> have found that fluid behavior in micro-systems is quite different than in similar systems of conventional scales. For flow in a micro-channel less than 20 microns wide, the resistance to fluid motion or the fluid's apparent viscosity is consistently smaller than that predicted by conventional, incompressible theory. For liquids, the apparent viscosity, inferred from the flow measurement, decreases with decreasing channel width. So far no explanation has been found to help in the understanding and modeling of these microscopic flows.

In manufacturing processes such as coating, fabrication of metal/ceramic composites, integrity of a solder joint, and containment of molten alloys, a detailed understanding of the interfacial reactions between liquid and solid substrate is required. Current continuum models that are used to predict the wetting behavior of liquids have been developed for aqueous and other simple liquid systems that assume either equilibrium conditions or minimal liquid/solid interfacial interactions. These continuum models are unable to predict wetting/de-wetting phenomena for non-equilibrium systems. It is suspected that in these systems, molecular-level interfacial processes, such as eutectic formation, interfacial inter-diffusion, corrosion induced roughening and alloy segregation, can control the interfacial energy and viscoelastic properties at the liquid/solid interface.

### 1.1 Technical Issues

For over a century, the Navier-Stokes equations with a given boundary condition have been successfully modeling the low-Reynolds-number flow of Newtonian fluids. However for a few fluid flow problems such as flow under high stress and flow in micro-domains, questions concerning the appropriate boundary conditions (BC) at solid surfaces and fluid interfaces have been raised. Specifically, the concern is about the commonly imposed no-slip boundary condition at a solid surface. Most past and present fluid mechanics research has shown an overwhelming phenomenological evidence that supports the no-slip condition at the solid surface<sup>9</sup>. Yet theoretically, there is not a well-established compelling

argument that totally supports a no-slip condition. According to the kinetic theory of gas dynamics, no-slip condition implies that for a stationary surface, the statistical average tangential component of the velocity of fluid molecules will be vanished after interacting with the solid molecules.

Maxwell<sup>10</sup> is the first to conduct a quantitative theoretical study of the no-slip condition by analyzing the interaction of dilute gas molecules in the presence of an idealized solid surface. By considering the specular reflection (a perfectly elastic collision between fluid molecules and solid molecules) as well as the diffuse reflection (an inelastic collision), Maxwell demonstrates that the average tangential velocity at the wall,  $u_{\text{wall}}$ , can be related to the shear rate,  $(\partial u)/(\partial z)$ , as

$$u = \lambda \frac{\partial u}{\partial z} \quad \text{(velocity at the wall and } z \text{ is normal to surface)}$$

where the slip-length,  $\lambda$  is given by

$$\lambda = \frac{2}{3}(2/f - 1)l$$

where  $l$  is the mean-free path of the gas molecules and  $f$  is the probability of diffuse reflection.

For a dilute gas under a very low pressure condition, the mean free path can become large; this leads to the Knudsen flow regime and the rarefied flow - slip condition. This theory predicts well the slip condition at the solid surface. However if the fluid is liquid, in which the mean free path is comparable to the molecular size, its slip length is almost equal to zero. According to the Maxwell theory, it is unlikely that slip condition will exist for liquid flow at a solid surface. Yet slip condition does exist in a few liquid flow problems such as the spreading of a liquid droplet and coating flow.

Imposing a no-slip or slip condition is one of the requirements when solving the Navier-Stokes equations. This continuum approach has always been applied as a macroscopic description of the fluid behavior. However under a certain condition, a microscopic phenomenon may become dominant that they influence the outcome of the fluid behavior. In that situation, it should be adequately modeled. Molecular dynamic simulations can be a reliable technique that will provide a valuable missing information.

When studying microscale fluid transport phenomena, one common question is: At what length scale does the continuum and equilibrium theory breaks down? If the continuum and equilibrium assumption fails, how does the fluid behave at the micron scale and what is the dominant physical mechanism? On the experimental side, a critical issue is how to design diagnostic techniques to investigate the microscale fluid transport phenomena and to measure properties at the micron or submicron scale. On the computational side, the important issue is how to model and characterize the flow properties at the micron scale. Figure 1 illustrates the existing simulation and modeling

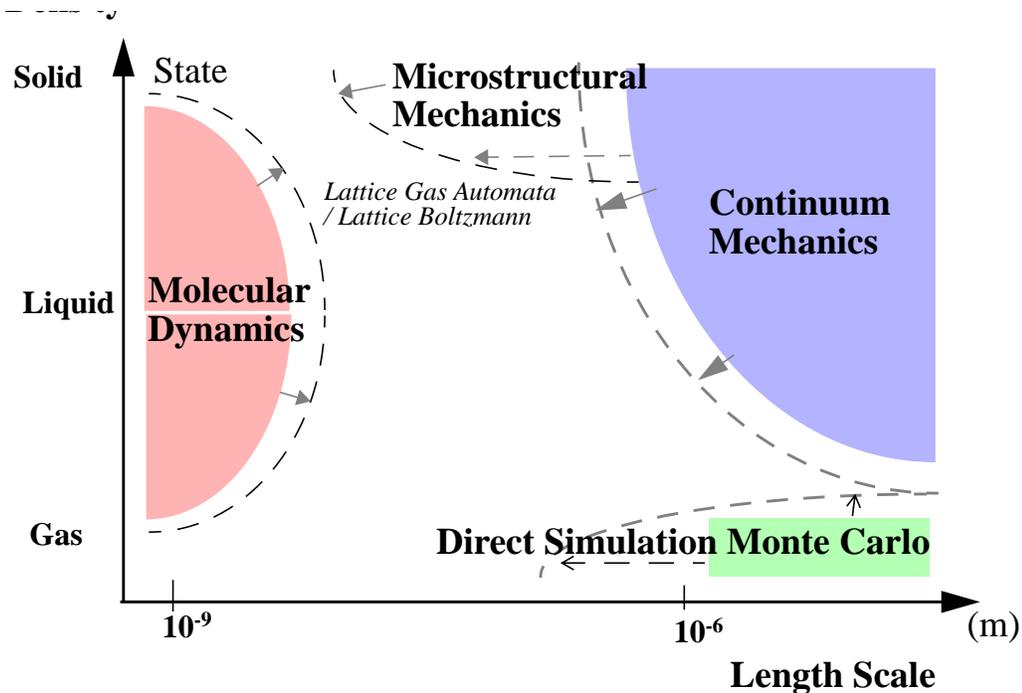


Figure 1. Simulation and Modeling Methodologies for Different Length Scales.

methodologies to analyze fluid transport phenomena at different length scales. At length scale larger than  $50\ \mu\text{m}$ , existing continuum theory works well. Bulk phenomena are dominant. On the other scale, at the atomistic and molecular levels, lattice dynamics in solid state physics<sup>3</sup> and molecular hydrodynamics<sup>4</sup> are the well-established methodologies to study different physical phenomena. However in the mesoscopic and microscopic scales, it is not clear what techniques or methodologies work best in this region. It has been shown that the traditional continuum and equilibrium theory is questionable<sup>5</sup>. For example, in structural dynamics and nonlinear mechanics, researchers have been using material particle approach (particle-in-cell method, element free Galerkin method, material point method, etc.) compliment to finite element techniques to investigate delamination of polymers and cracking of solder joints<sup>6</sup>. For gas dynamics at a low pressure or in a micro-domain, Direct Simulation Monte Carlo (DSMC) is being used to model this rarefied gas transport<sup>7</sup>. Lattice Gas Cellular Automata and Lattice Boltzmann techniques are being developed and applied to analyze flow in porous media<sup>8</sup>. There are many other active research going on in microscale fluid transport.

Our project is to focus on the modeling issues by utilizing molecular dynamics simulations to better understand the transport phenomena at a micron scale. In addition to use for model development, MD simulation is also needed to design experiment to diagnose micro-transport mechanisms.

## 1.2 Molecular Dynamics Simulations

Simulations at the molecular level can provide insight to identify the dominant microscale physics so that it will help us to develop macro-models and constitutive relationships. Molecular dynamics simulations involve: (1) specifying an intermolecular potential, (2) integrating Newton's equation of motion for a large number of interacting molecules comprising a volume of fluid and for a sufficiently long molecular time scale, and (3) deriving the macroscopic transport properties from the microscopic information of the dynamic motion of the molecules. Since the characteristic scales at the molecular level are small, each simulation requires a very large number of molecules and many time steps in order to produce a reliable solution for a problem of interest. Thus, the drawback of molecular level simulations is that it is very computationally intensive. One primary task of our project is to analyze fluid flow and structure interaction at the molecular level. The ultimate physical domain of interest will be about 5  $\mu\text{m}$  by 5  $\mu\text{m}$ .

Our strategy is to further developing a molecular dynamics (MD) computer program<sup>11,12</sup> for fluid transport analysis. This is needed because the existing MD program is designed for macro-molecular systems such as polymers and proteins. Our interests include: (1) to define the slip conditions at the boundary, (2) to investigate the effect of scale, and (3) to develop macro-transport coefficients such as anisotropic viscosity. This area of research is relatively new, unique, and innovative.

Molecular dynamics (MD) simulations solve the classical equations of motion of a molecular system. At the simplest level this is just integrating Newton's equation for a system of  $N$  atoms. For a Cartesian coordinates, the Hamilton's equations of motion can be expressed as follows:

$$\dot{r}_i = p_i/m_i$$
$$\dot{p}_i = -\nabla V = f_i$$

where  $m_i$  is the mass,  $p_i$  is the momentum,  $f_i$  is the force, and  $V$  is the interaction potential.

The major input in an MD program is the initial position, velocities and identity of each atom, and the forces between the atoms. The basic forces include those of class I: van der Waals, Coulomb, bond stretch, bond bending and torsion. Force fields of class II involve cross terms between class I forces.

The LAMMPS (Large Atomic/Molecular Massively Parallel Simulator)<sup>13</sup> molecular dynamics program can treat systems described in terms of Class I potentials and Class II potentials. The parallelization is done by a spatial decomposition; atoms are allocated to processors by assigning each processor part of the system space. LAMMPS can treat various ensembles including constant temperature and constant pressure. A variety of constraints are also available. For example, walls can be defined as a set of atoms which do not move.

The particle dynamics is integrated by the Verlet algorithm which is a simple finite difference scheme. It involves two half time step velocity steps with a full time step position step in between. One advantage of the Verlet algorithm is that the force is only evaluated once. This is essential since the force calculation usually comprises 90% of the computational time. Another advantage is that the algorithm is symplectic and is more stable than for classical dynamics than nonsymplectic methods such as predictor-corrector.

### 1.3 Previous Work

Defining the boundary conditions at the solid surface is essential to analyze fluid flow problems. In many problems, no-slip boundary conditions has been used; this implies that the tangential component of the fluid velocity at the boundary is equal to the surface wall velocity. While in most cases, implementing a no-slip boundary conditions is valid, in other cases such as lubrication flow, flow in porous media, and the spreading of fluids, the no-slip boundary conditions become questionable. Much work have been done to define a better slip boundary condition via macroscopic/continuum approach. However no satisfactory physical model has been found.

Recently microscopic analyses such as non-equilibrium molecular dynamic simulations of simple fluids have been used to study fluid flow near solid surfaces. Koplik<sup>14</sup> and Evan<sup>15</sup> present excellent review of the work in this area in the past decade. Most of the work involve studying ideal Poiseuille and Couette flow as well as flow through small pores. In the early studies, various types of structureless walls are used and only slip boundary conditions are predicted<sup>16</sup>. In the past decade, more realistic simulations were performed. The wall modeled is composed of atoms arranged on a lattice; results of these simulations revealed more complex boundary conditions. Under very confined conditions, locking between wall and fluid was observed<sup>17-19</sup>. Locking implies that the fluid within one or two molecular spacing adjacent to the wall processed with the same velocity as the wall surface. Heinbuch<sup>19</sup> and Thompson<sup>17</sup> found that this locking distance increased with the strength of wall-fluid interactions and decreased with temperature. This findings have also been verified by experiments<sup>20,21</sup>, showing a variety of boundary conditions may occur, ranging from locking to slip.



## 2. MD Code Development and Wall/Fluid Atoms Modeling

The molecular dynamics (MD) code upon which development was done is the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) program<sup>13</sup>. The LAMMPS program is a general purpose massively-parallel MD code. It runs on a variety of parallel computers, including NCube, Paragon, and T3D/E, and it can be run on unix workstations.

LAMMPS can perform atomistic simulations using realistic potentials or perform model simulations. Examples of applications are nylon flow, liquid crystals, and bio-membranes. The original force field was the CHARMM force field. This includes the various molecular potentials: bond stretching, bond bending, and torsion. Extensions to the Class II Biosym force field are presently being inserted. Besides realistic potentials, one can also treat model systems. In addition, Lennard-Jones interactions are treated with full variability of the coefficients of the  $r^6$  and  $r^{12}$  terms (Fig. 2). Long ranged Coulomb interactions are treated using the particle-mesh Ewald algorithm.

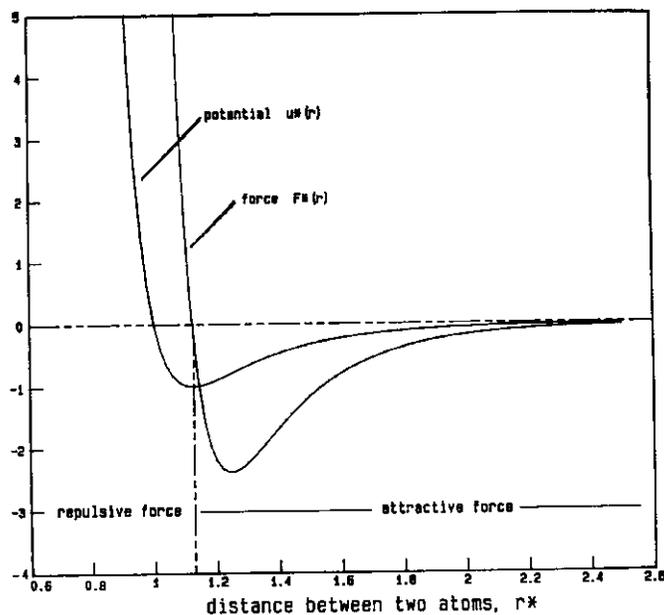


Figure 2. Schematic Diagram of the Lennard-Jones Potential

In order to treat flow problems various additions were made to LAMMPS. To treat flow in a channel, walls were introduced. The walls are explicitly described by particles which can be constrained in various ways. In the basic stationary wall, the wall atoms are constrained to their original positions. The original positions are determined by a separate

program that creates the initial configuration (mkinp program). In most cases, the wall structure has been a fcc lattice. The wall atoms may be allowed to move about their lattice sites such that the wall is constrained to be at some input temperature. In this manner, the heat transport between walls can be modeled.

To simulate flow, the flow must be induced in some manner. There are multiple means that we have implemented. To simulate Couette flow, a fluid is placed between two parallel walls. The top wall is pulled at a constant velocity. The interaction between the wall and the fluid causes the fluid to flow. A linear velocity profile will form with boundary conditions that depend on the wall-fluid interaction, the fluid density, the temperature, etc. (see Chapter 4). To produce Poiseuille flow, we mimic Poiseuille flow induced by gravity. The same parallel wall setup is used as is for Couette flow. An added force is applied to each atom while keeping the walls stationary.

Once there is flow in the system, calculating the temperature requires special treatment. The temperature is related to the kinetic energy. In calculating the kinetic energy, the velocity of the particle used should be the peculiar velocity or the total velocity minus the flow velocity.

For analysis, two important quantities must be calculated. One is the flow profile which must also be calculated when thermostating the fluid. This is determined by binning the particles in layers perpendicular to the walls. The layer thickness is about the diameter of a particle. Then the average velocity is calculated to be the flow velocity at that layer. Another important quantity is the shear stress which can be determined from the force on the walls. Knowing the stress one can then calculate the viscosity using the flow profile to get the shear rate.

## 3. Code Assessment

### 3.1 Key Issues with Assessing MD Simulations

Molecular dynamics simulations of liquid motion is a unique approach to investigate fluid transport. It starts with the microscopic simulation of a system (the masses of atoms or molecules, the interaction between them, molecular geometry, etc.) and ends with macroscopic properties of interest (the equation of state, transport coefficients, structural order parameters, and so on). These macroscopic properties are derived from statistical averaging of the dynamics of the molecular system. To assess the results of the MD simulations, we need to be aware of the following important issues, that are quite different from those involved in traditional computational fluid dynamics simulations based on continuum mechanics.

#### 1. Validating and verification the code predictions

There are few important areas that are very helpful in assessing the predictions from the MD simulations. By following this routine, one can easily build up the confidence and reliability of the simulations.

- **Equilibration** - During the equilibration process, before any velocity scaling, the total energy should remain constant. Then at the end of the equilibration, the positional order parameter should fluctuate about zero and the H-function should be consistent with Maxwell velocity distribution.
- **Conservation** - Simulations should obey these conservation laws: (a) number of simulation particles remains constant with time, (b) total linear momentum at each Cartesian coordinate is zero, and (c) total energy is constant with time.
- **Properties** - Review the behavior of the predicted properties. For example, kinetic energy should have an equal quantity amongst different components. Under equilibrium conditions, the predicted properties for an instantaneous time interval should be relatively stable, do not fluctuate much, and give reproducible results.

#### 2. Minimizing the statistical error

For the production run, it is very important to divide a computed phase-space trajectory into segments whose durations are longer than the relaxation time. This will minimize any statistical error.

#### 3. Systematic error

Check out the systematic errors, those general behavior of different properties derived from the simulations. For example, watch out for the drift in total energy or running average for properties. It is also very helpful to check for normal distribution and thermodynamic limit. They usually give good insight into the accuracy of the predictions.

#### 4. Independent tests

It is useful to perform independent tests. This involves repeating simulations in different computing environments like different computers, different compilers, different algorithms, or different simulation methods.

### 3.2 Comparison with Other MD Simulations of Couette Flow

This section will discuss our development and assessment effort to simulate flow between solid walls using molecular dynamics (MD) approach. Our simulation effort involves developing programs (e.g. mkinput program in Appendix A) to create initial and boundary states of the molecule structures and applying the MD technique to simulate fluid motion for the microscale Couette and Poiseuille flow problems. Simulation at the molecular level is crucial in determining the boundary condition (e.g. stick or slip) at the fluid-solid interface. This boundary condition (BC) is prescribed using ad hoc empirical approaches in continuum theory, but is an important input in continuum calculations.

The first class of simulated fluid flow problems is microscale Couette flow. To model the microscale Couette flow, we have the problems set up such that the upper wall is moving to the right with a dimensionless velocity of 2 (Figure 3). Velocity is normalized and expressed in term of the reduced LJ units (i.e.  $v^* = v \sqrt{m/\epsilon} = 2$ , where  $m$  is the mass of the molecule and  $\epsilon$  is the characteristic interaction energy of the Lennard-Jones (LJ) fluid). Unlike the upper wall, the lower wall is stationary ( $v^* = 0$ ). The lattice structure of both upper and lower walls is face-centered cubic (fcc) crystal. The fluid is being sheared between the (001) surfaces of the fcc crystal. The separation distance between two walls is  $12.8\sigma$ , where  $\sigma$  is the a characteristic diameter of the molecule (the “collision diameter”). For most molecules,  $\sigma$  is about a few Angstroms, depending on the size of the molecule; usually it spans from  $\sim 2.5$  to  $5 \times 10^{-10}$  m.

In this study, total number of particles simulated is 864, with 672 representing the fluid particles and 192 representing the wall particles. Since our interest is to investigate the effect of different wall-fluid interactions on the fluid motion, these simulations will have both fluid and wall having the same density of 0.81 and the same temperature (isothermal

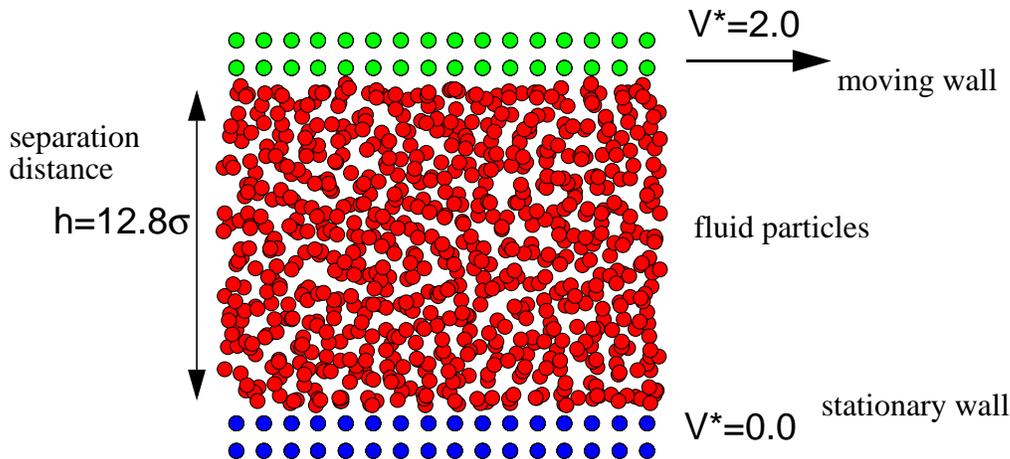


Figure 3. Layout of the Fluid and Wall Particles in the MD Simulations of the Couette Flow.

and adiabatic problem) of 1.1, i.e.  $\rho^* = \rho\sigma^3 = 0.81$  and  $T^* = k_b T / \epsilon = 1.1$ , where  $k_b$  is the Boltzmann constant. Three different degrees of wall-fluid interaction have been studied:  $\epsilon_{wf} = 0.4, 1.0,$  and  $4.0$ . The larger the value, the stronger the wall-fluid interaction will be.

Similar to other MD simulations performed by Thompson, et al.<sup>17,18</sup>, our MD results show that slip BC, i.e. a jump in the velocity profile at the fluid-wall interface, will occur if the interaction between the fluid and wall molecules is weak (Fig. 4). Specifically the ratio of the pair interaction potential in this study,  $\epsilon_{wf}/\epsilon_{ff}$ , is set at 0.4, where  $\epsilon$  is the characteristic interaction energy of the Lennard-Jones (LJ) fluid.

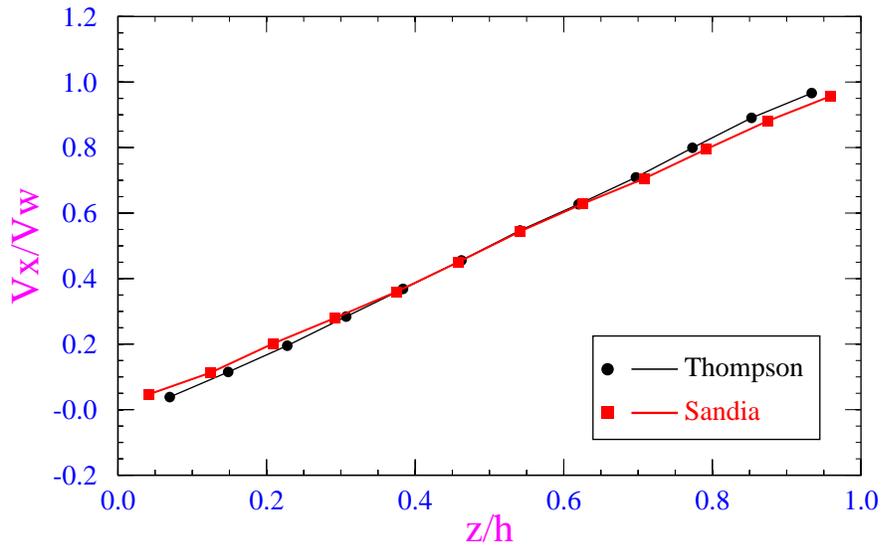


Figure 4. Velocity Profiles of Microscale Couette Flow for Wall-Fluid interaction Potential Equals to 0.4

For the conditions in which the wall-fluid interaction equals to the fluid-fluid interaction, i.e.,  $\epsilon_{wf}/\epsilon_{ff} = 1.0$ , no-slip BC will occur at the fluid-solid interface and the fluid velocity profile is linear between the walls (Fig. 5). This linear behavior is consistent with the prediction from the classic continuum fluid mechanics.

An interesting finding exists when there is a strong wall-fluid interaction,  $\epsilon_{wf}/\epsilon_{ff} = 4$ . The stick BC, i.e. fluid layers adjacent to the walls, are being locked with the solid wall, is predicted (Fig. 6). This leads to a nonlinear velocity distribution between the walls and a higher apparent viscosity than expected. This finding of stick boundary condition, which is very different from the classic fluid mechanics theory, has been observed in many experimental measurements<sup>20,21</sup>. These unique features, slip BC as well as stick BC, can

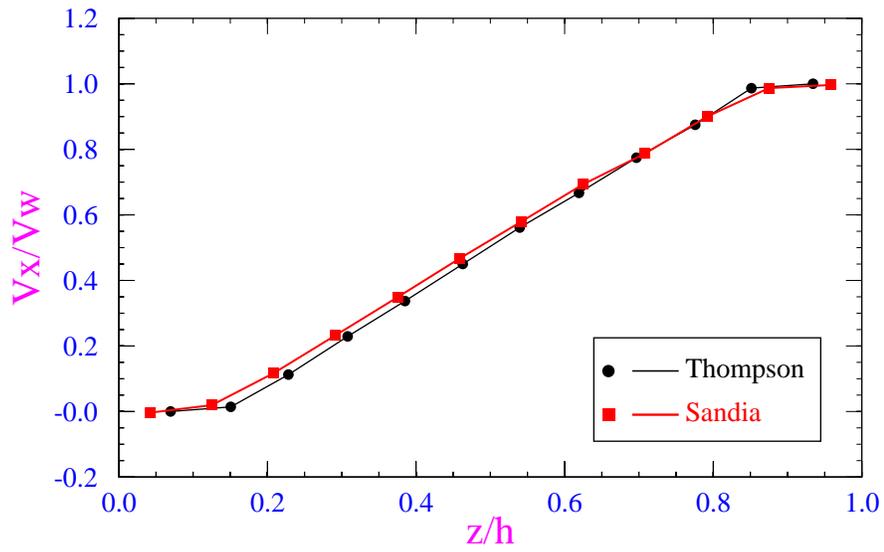


Figure 5. Velocity Profiles of Microscale Couette Flow for Wall-Fluid Interaction Potential Equals to 1.0

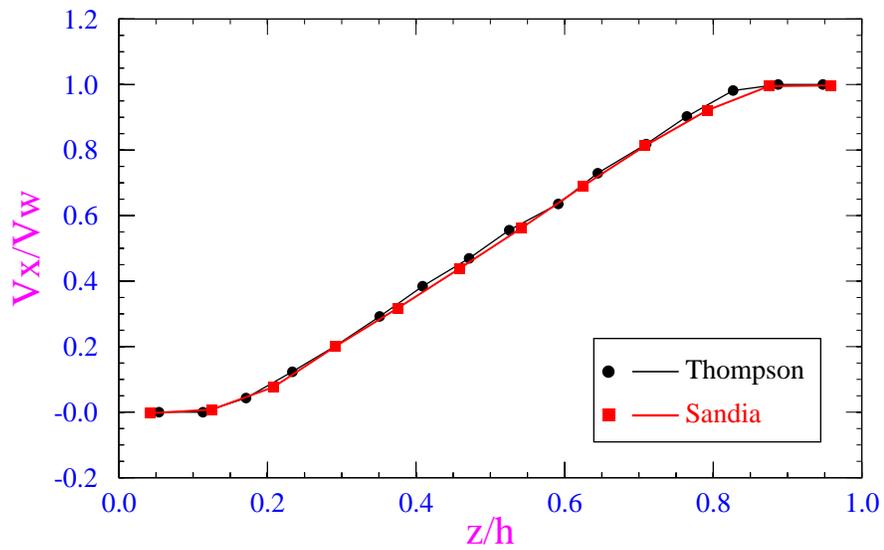


Figure 6. Velocity Profiles of Microscale Couette Flow for Wall-Fluid Interaction Potential Equals to 4.0

easily be predicted with MD simulations. In the continuum approach, it is very unclear what BC should be used when solving the Navier-Stokes equations to analyze these kinds of problems. With a no-slip BC, it will only yield a linear velocity profile across the channel, thus it fails to model the wall-fluid interaction accurately.

### 3.3 Comparison with Other MD Simulations of Poiseuille Flow

The second class of fluid flow problems that we have studied are the microscale Poiseuille flow problems. The setup and layout of the fluid and solid molecules is similar to the Couette flow problems in Section 3.2. Both walls have a fcc crystal structure with the (001) plane representing the fluid-solid interface, as in Fig. 7. The separation distance has been reduced to  $11\sigma$  such that our simulations are consistent with other MD simulations performed by Koplik<sup>22,23</sup>. To model the pressure gradient along the microchannel, a uniform acceleration ( $g^*=0.1$  expressed in reduced units of the Lennard-Jones system) parallel to the walls has been applied to all fluid molecules.

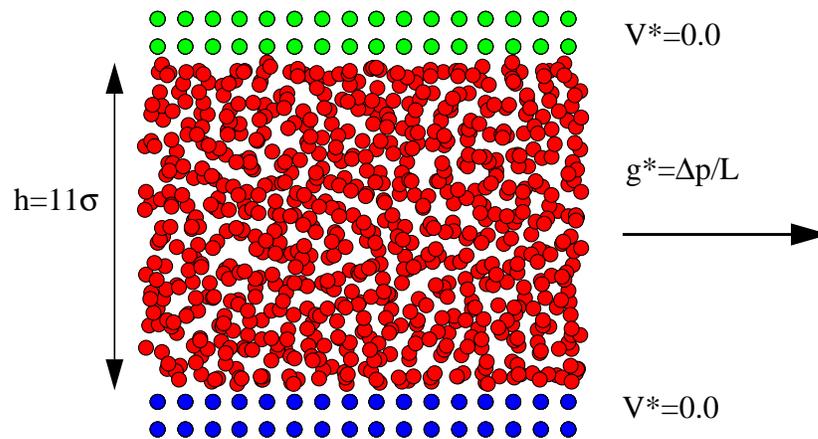


Figure 7. Layout of the Fluid and Wall Particles in the MD Simulations of the Poiseuille Flow

Other boundary conditions are set up as follows: since this is an isothermal and adiabatic flow, both fluid and wall temperature are set at 2.5 ( $T^*=k_B T/\epsilon=2.5$ ). The wall-fluid interaction,  $\epsilon_{wf}$ , remains constant at 1.0. The wall density ( $\rho^*=\rho\sigma^3$ ) is kept constant at 0.8, however three different fluid densities (0.4, 0.6, and 0.8) have been simulated. This assessment exercise is to further validate our MD code's capability to study rarefied effect.

Our MD simulation of the pressure-driven flow in a microchannel with the (001) wall and fluid density of 0.8 produce a parabolic velocity profile that agrees with the analytical predictions by solving the Navier-Stokes equation with no-slip boundary condition (Fig. 8). However for other cases with fluid densities of 0.6 and 0.4, our MD simulations indicate

that there exists a slip BC and it changes the velocity profile. This implies that for a constant pressure head, flow in a narrow microchannel with a less density fluid ( $\rho^*=0.4$ ) will have a larger maximum velocity and a smaller apparent viscosity than flow in a microchannel with a fluid density of 0.8. This finding is consistent with Koplik's results (Table 1).

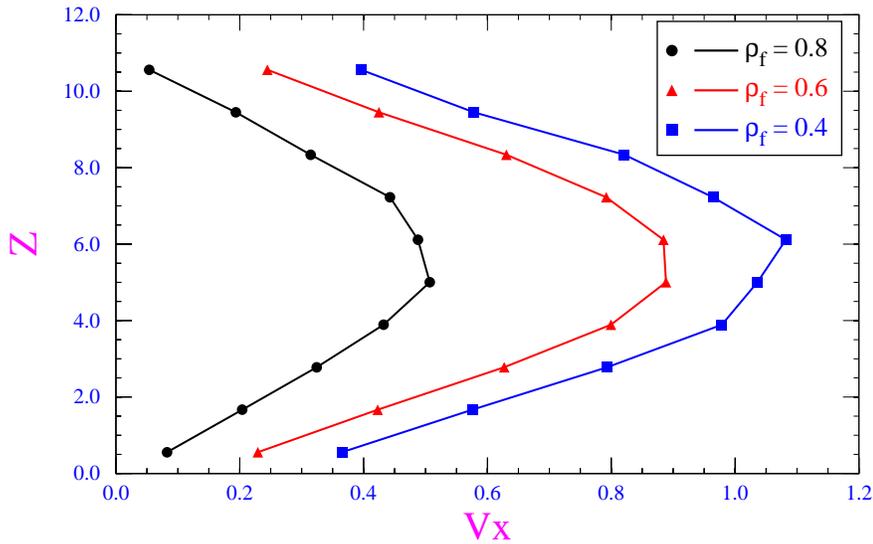


Figure 8. Velocity Profiles of Microscale Poiseuille Flow for Different Fluid Densities with Wall-Fluid Interaction Potential Equals to 1.0

$\rho$	$V_{\max}$	Koplik ( $V_{\max}$ )	$\mu$	Koplik ( $\mu$ )
0.8	0.51	0.50	2.47	$2.04 \pm 0.40$
0.6	0.89	0.80	1.04	$1.04 \pm 0.15$
0.4	1.08	0.95	0.57	$0.67 \pm 0.08$

Table 1. Comparison of the Present Code Predictions with Predictions from Koplik for the Poiseuille Flows

## 4. Microscale Couette flow

In the previous sections, we have presented the results of our MD code predictions of the microscale fluid flow problems. Its comparisons against other MD simulations are excellent. Most of these findings such as the stick-slip conditions have been observed in various experiments and can be used to explain many unexpected physical phenomena that appear in the micro-domains. After the assessment exercise, the next sets of simulations will focus an important issue to determine at what length scales that the breakdown of the continuum mechanics will occur. Hence our approach to investigate the size effect is: (1) to qualify more about the wall-fluid interaction by exploring other lattice structures of solid atoms, and (2) to determine when the stick-slip phenomena or surface effect becomes less important by increasing the separation distance between walls. Both studies are relatively new and have not been well-addressed yet.

### 4.1 Effect of Lattice Structure of Solid Atoms

Previous studies on microscale Couette flow have imposed a boundary such that the fluid is being sheared in the  $\langle 1,0,0 \rangle$  direction and along the (001) planes of the fcc walls. The (001) plane is relatively easier to set up and visualize what happens. In addition, the overall interaction between fluid and wall molecules for this arrangement is the strongest because of the lattice orientation. However other shear direction and plane has not been investigated and reported. In our study, we have the fluid being sheared along a different direction, the  $\langle 1,1,-2 \rangle$  direction and along a different plane, the (111) plane. These two surface structures are quite different as shown in Fig. 9.

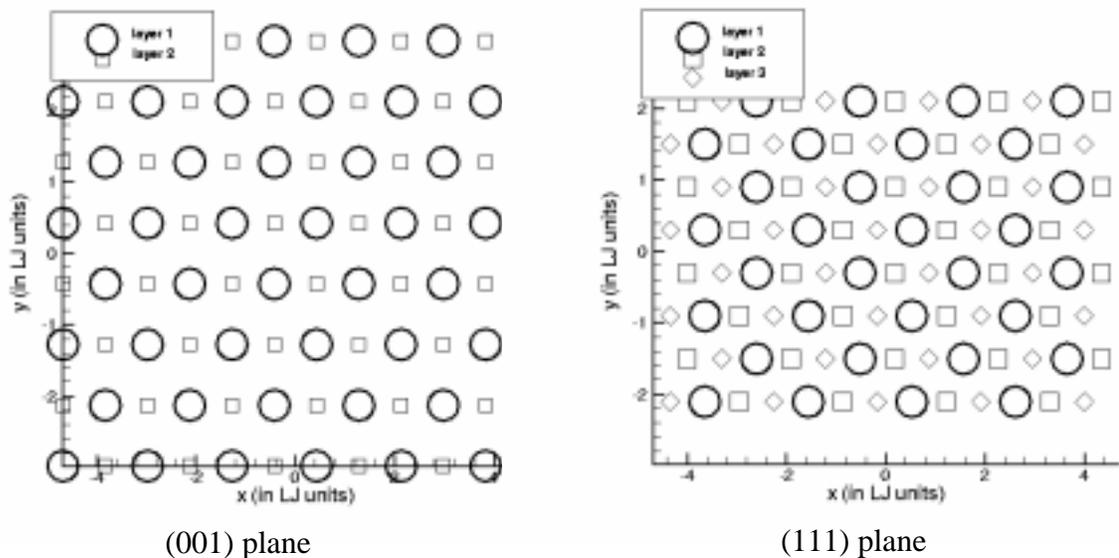


Figure 9. Surface Topology of the (001) Plane and the (111) Plane of the FCC Crystal.

Our results shows that shear direction with respect to the wall lattice orientation is important. For the case with a strong wall-fluid interaction ( $\epsilon_{wf}/\epsilon_{ff}=4$ ), unlike Thompson's findings<sup>4</sup>, our MD simulations show that the velocity profile will be different for two different kinds of lattice orientation of solid atoms, (001) wall versus (111) wall (Fig. 10). The solid atoms in the (111) wall are close-packed and is smoother than the (001) wall. Hence the overall wall-fluid interaction is reduced because of the closely packed lattice structure. Thus the velocity profile is more linear. This discovery is relatively new and unexpected. Information like this is very helpful to the designers that deal with micro-systems in which the surface phenomenon becomes very important.

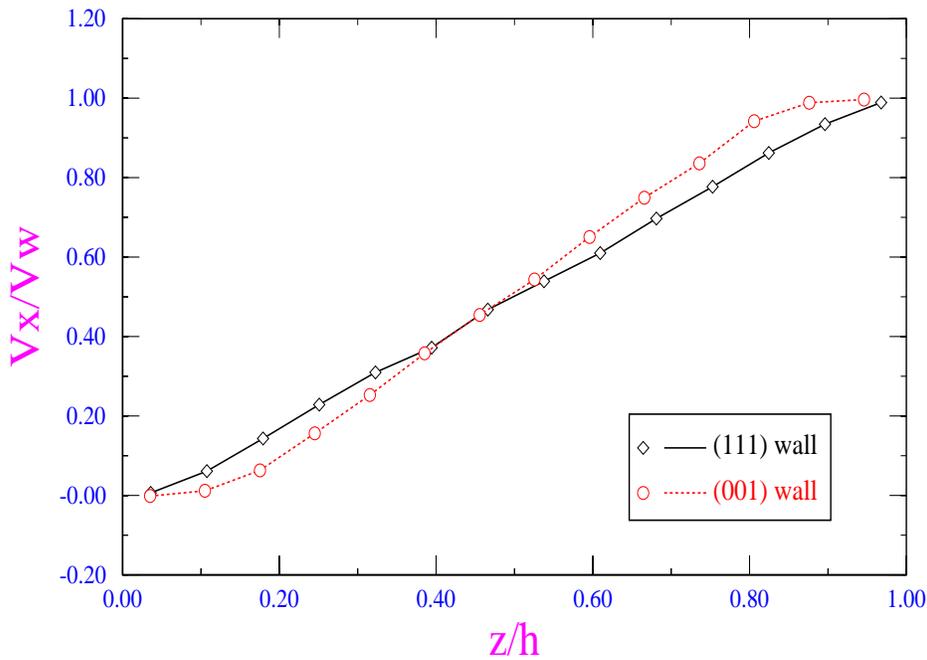


Figure 10. Velocity Profiles of Microscale Couette Flow Problems with Different Atom Structures at the Wall.

## 4.2 Effect of Separation Distance

The effect of plate separation on the stick boundary conditions (BC) has also been investigated. These simulations have the microchannel widened from  $12.8\sigma$  to  $128\sigma$  and study the changes in the velocity profile (Fig. 7). This implies that if the working fluid is liquid Argon, the separation distance will increase from 2.5 nm to 25 nm. As the separation distance increases, the channel is wider. Many more particles are needed to simulate the fluid transport between the walls. Hence we have to conduct these MD simulations in a massively parallel computing environment, specifically the MD code is run on the 1024-node NCube machine.

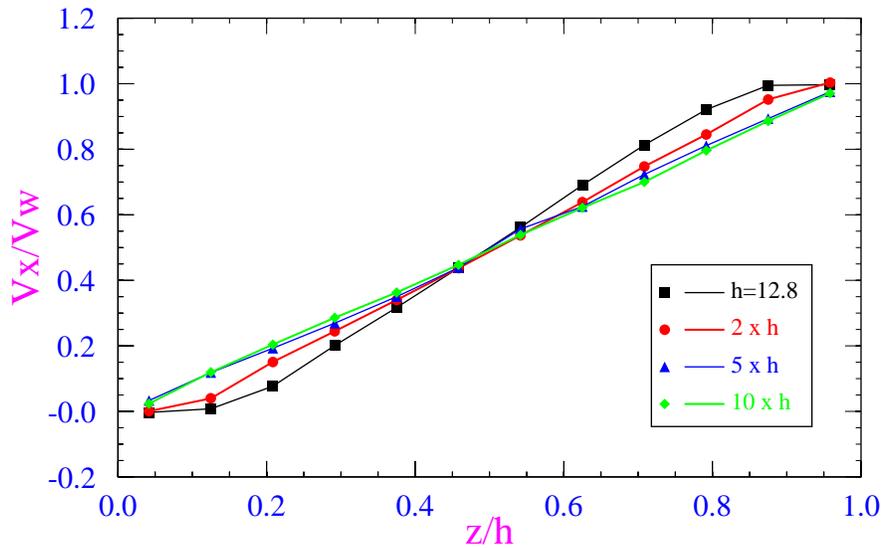


Figure 11. Velocity Profiles of Microscale Couette Flow for Different Separation Distances with Wall-Fluid Interaction Potentials Equal to 4.0

The results of this length-scale study are quite interesting. As the channel size increases, the velocity profile becomes more linear. It behaves just like the analytical solution of the classic continuum mechanics theory. If zooming into the wall-fluid interface and taking a closer look at the fluid behavior adjacent to the wall, for a wider channel, locking still occurs in a few fluid layers adjacent to the wall. However its effect is minimal for the widest microchannel. Hence this locking behavior does not depend on the plate separation and it is always there. Since the effect of wall-fluid interaction on the bulk fluid is more dramatic for the narrower channel, one needs to model this interaction accurately. As to determine the breakdown length-scale, our analysis indicates that the surface effect becomes more dominant than the bulk effect when the channel width is less than  $60\sigma$ , i.e., at about 12 nm for liquid Argon as the working fluid.



## 5. Microscale Poiseuille flow

Besides analyzing the microscale Couette flow as in the previous chapter, we have also investigate the effect of lattice structure and the effect of separation distance on the fluid behavior for the Poiseuille flow problem. Again the pressure gradient along the micro-channel is modeled as a global potential applied uniformly to each fluid particle ( $g^*=0.1$  expressed in the reduced units of the Lennard-Jones system). Hence this potential will generate a uniform force field parallel to the walls representing pressure head that drives the fluid to flow downstream along the microchannel.

### 5.1 Effect of Lattice Structure of Solid Atoms

For a better comparison, we have our MD simulations set up to be consistent with earlier simulations in section 3.3. Thus these MD simulations are imposed with an interaction pair potential between the fluid and wall being the same as the interaction pair potential between the fluid and fluid. Early results (in section 3.3) shows a parabolic velocity profile exists between the channels, similar to the predictions from the classic continuum mechanics theory. However if there is a strong interaction between the wall and fluid ( $\epsilon_{wf}/\epsilon_{ff}=4.0$ ), will the stick condition, where those fluid layers adjacent to the wall are locked with the solid molecules, still exist? Our MD result show that stick condition does exist at the fluid layer adjacent to the wall (i.e. represented by the solid line in Fig. 12).

With different lattice structures of solid walls, our MD simulation of pressure-driven fluid flow in a microchannel also indicates that the velocity profile will behave differently. For the (111) wall, it produces a parabolic velocity profile that agrees with the analytical predictions obtained by solving the NS equations with a no-slip boundary condition (Fig. 12). However for a microchannel with the (001) wall, our MD simulations indicate that there exists a stick BC and it changes the velocity profile. This implies that for a constant pressure head, flow in a very narrow microchannel with a (001) wall will have a smaller maximum velocity and a larger apparent viscosity than flow in a microchannel with a (111) wall. This information is very important to MEMS researchers when fabricating silicon wafers for microchannels in the development of micro-devices like a chem-lab on a chip or a micro bio-analyzer or to nano-machine researchers when building carbon nanotubes for nano-systems.

### 5.2 Effect of Separation Distance

The effect of wall separation distance on the stick BC in the microscale Poiseuille flow is similar to the microscale Couette flow (Fig. 9). We have simulated the pressure-driven fluid motion for two additional problems with two different channel sizes. As the micro-channel gets wider, many more fluid particles are needed for simulations. These simulations are performed in a massively parallel computing environment. Results from our simulations show that for a wider channel, the effect of wall-fluid interaction on the bulk fluid is less dramatic than the narrow channel. Locking still occurs in a few fluid layers adjacent to the wall (Fig. 10) and it does not depend on the wall separation distance. This implies that surface phenomenon as wall-fluid interaction becomes more important than

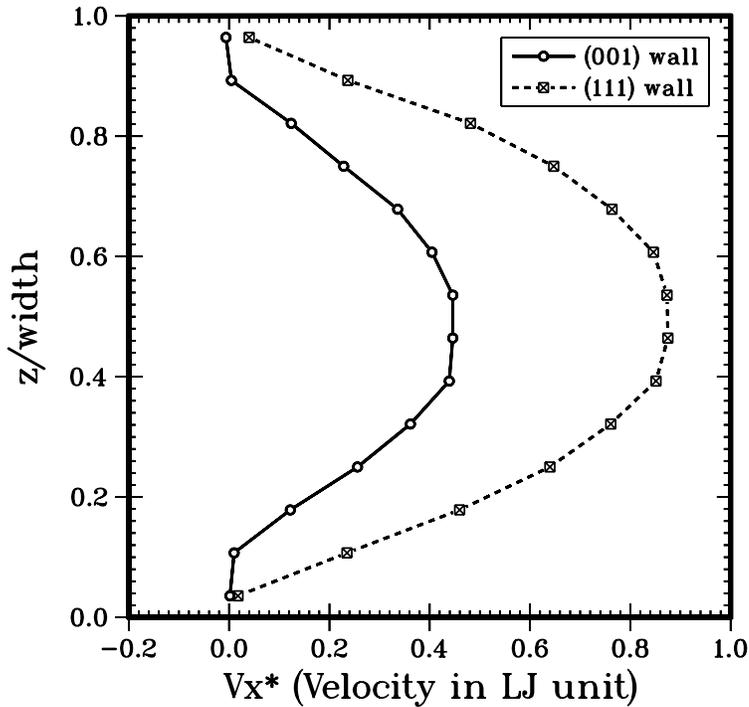


Figure 12. Velocity Profiles of Microscale Poiseuille Flow Problems with Different Atomic Structures at the Wall.

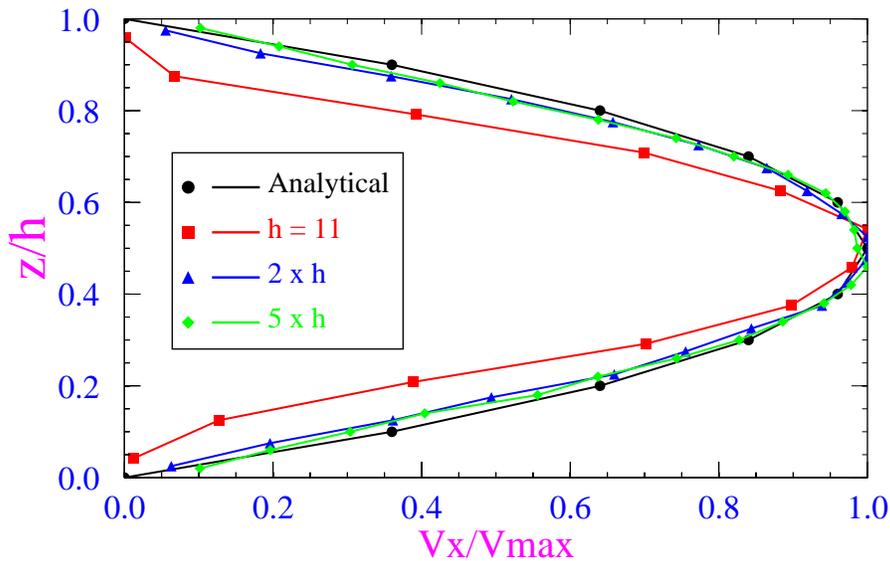


Figure 13. Velocity Profiles of Microscale Poiseuille Flow for Different Separation Distances with Wall-Fluid Interaction Potentials Equal to 4.0

the bulk effect as the microchannel size decreases. However this influence will not be significant until the separation distance is about  $2\sigma$ , i.e. about 5 nm for the liquid Argon flow.

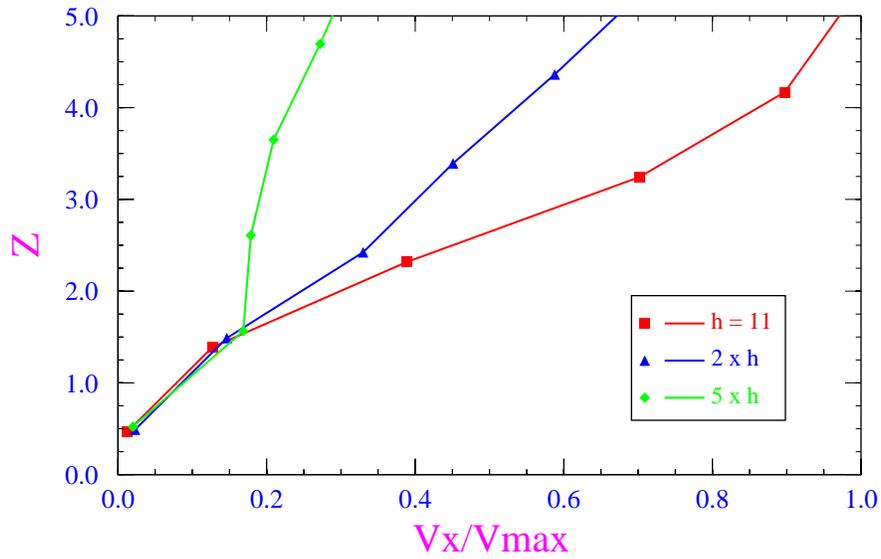


Figure 14. Velocity Profiles of Microscale Poiseuille Flow for Different Separation Distances but with Wall-Fluid Interaction Potentials Equal to 4.0



## 6. Conclusions and Recommendations

Technology advancement in MEMS and in many manufacturing processes such as coatings, has generated a group of unique fluid flow problems that involve characteristic length scales of a micron. Current continuum models are unable to predict microscale physical phenomena that appear in these non-equilibrium systems. To address these microscale fluid transport problems, we have developed and assessed a massively parallel molecular dynamics (MD) code to better understand microscale transport mechanisms, fluid-structure interactions, and scale effects in micro-domains. Specifically, this MD code has been used to analyze liquid channel flow problems for a variety of channel widths and solid surface structures. Results from these MD simulations of Poiseuille flow and Couette flow problems have demonstrated that in these micro-systems, molecular-level processes can control the interfacial energy and viscoelastic properties at the liquid/solid boundary. MD simulation is a powerful technique for these microscale transport problems.

Even though these MD simulations of microscale Couette and Poiseuille flow problems have demonstrated the importance of this technique to help understanding fundamental microscale hydrodynamic phenomena, more work is still needed to further develop and validate this methodology. One area that we have worked on is to couple the atomistic approach with the continuum approach to study fluid transport problems that involve multiple length-scales. We have developed and demonstrated a coupling strategy for these multi-length scale problems. The results of these coupling work are very encouraging and will be published in a separate report. The other area is to extend the current study to account for rough wall and to model complex fluids. This work has already begun. Our interest is to analyze more realistic, complicated interaction between wall structure and fluid that appear in MEMS or other micro-structures.



## 7. References

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# Appendix A: Listing of the mkinput Program

```
c  program mkinp.f    July 30, 1997
c....
c....  ifcc=1 for fcc (001) wall
c....  ifcc=2 for fcc (111) wall shearing in [1,1,-2] direction, x-dir
c....  ifcc=3 for fcc (111) wall shearing in [-1,1,0] direction, x-dir
c....
c....  MUST HAVE WALLS
c....
c....  Origin at (0,0,0)
c....  This program creates a hcpish configuration of a LJ molecular fluid.
c....  OR a LJ atomic fluid.
c....
c....  May have Walls!
c....  If walls, each wall has 2 layers of fcc. SHOULD BE GENERALIZED.
c....  for ithw=0 (stationary wall atoms),
c....      itype = 2 is bottom wall.
c....      itype = 3 is top wall.
c....  for ithw=1 (wall with thermally vibrating atoms),
c....      itype = 2 is lattice site of bottom wall.
c....      itype = 3 is initial atom location of bottom wall.
c....      itype = 4 is lattice site of top wall.
c....      itype = 5 is initial atom location of top wall.
c....
c....  Dimensions:
c....
c....  a_nn is nearest neighbor distance within a plane of wall
c....  lattice.
c....  nxw and nyw are the number of layers that make the wall
c....  crystal. They must be even!
c....  bond is the average bond length for the molecule.
c....  mx,my is the number of molecular cells in the x,y directions.
c....  mz is the number of layers in the z direction.
c....  fz is a scaling factor to alter the wall spacing.
c....
c....  for the (001) wall. i.e. ifcc=1
c....  hx = a_nn * sqrt(2) * mx * nbeads / 2
c....  hy = a_nn * sqrt(2) * my
c....  hz = a_nn * mz * fz * sqrt(2) / 2
c....
c....  for the (111) wall shearing in [1,1,-2] dir. i.e. ifcc=2
c....  hx = a_nn * sqrt(3) * mx * nbeads / 2
c....  hy = a_nn * my
c....  hz = a_nn * mz * fz * sqrt(6) / 3
c....
c....  for the (111) wall shearing in [-1,1,0] dir. i.e. ifcc=3
c....  hx = a_nn * mx * nbeads / 2
c....  hy = a_nn * sqrt(3) * my
c....  hz = a_nn * mz * fz * sqrt(6) / 3
c....
c....  nmax is the max total number of atoms

c234567890123456789012345678901234567890123456789012345678901234567890

parameter(z1=1.0,nmax=100000)
```

```

common/hmatrix/ hx,hy,hz,cellx,celly,cellz,fx,fy
common/hmatrix2/ hx2,hy2,hz2
common/numbers/ natom,nbeads,nsites,ifcc,ithw
common/fluid/ x0(nmax,3)
dimension xc(nmax),yc(nmax),zc(nmax)

ilat=0

110 continue
write(6,*) 'Please enter the desired layout of atoms/molecules'
write(6,*) 'Your choices are as follows:'
write(6,*) 'Enter 1 for fcc (001) lattice'
write(6,*) ' 2 for fcc (111) lattice with x-dir=[1,1,-2]'
write(6,*) ' 3 for fcc (111) lattice with x-dir=[-1,1,0]'
read(5,*) ifcc

go to (111,112,113), ifcc
write(*,*) 'ifcc must be less than 4. Try again, please.'
go to 110
111 xfp = sqrt(2.0)
yfp = sqrt(2.0)
zfp = sqrt(2.0) / 2.0
go to 115
112 xfp = sqrt(3.0)
yfp = 1
zfp = sqrt(6.0) / 3.0
go to 115
113 xfp = 1
yfp = sqrt(3.0)
zfp = sqrt(6.0) / 3.0
go to 115

115 continue

write(6,*) 'Number of beads per molecule?'
read(5,*) nbeads

if (nbeads.gt.1) then
96 continue
if (mod(nbeads,2).ne. 0) then
write(6,*) 'nbeads must be even. Try again, please.'
write(6,*) 'Enter nbeads '
read(5,*) nbeads
goto 96
end if
write(6,*) 'Bond length is 0.96.'
write(6,*) ' '

ilat = 1
write (6,*) 'Number of fluid layers =?'
read(5,*) mz
write (6,*) 'Scaling factor, f_z, for wall separation =?'
read(5,*) fz
write(6,*) 'No. of molecule cells in x & y direction: mx, my?'
read(5,*) mx, my
95 continue
if (mod(mx,2).ne. 0) then
write(*,*) 'mx must be even. Try again, please.'
write(*,*) 'Enter mx '

```

```

        read(*,*) mx
        goto 95
    end if
94  continue
    if (mod(my,2).ne. 0) then
        write(*,*) 'my must be even. Try again, please.'
        write(*,*) 'Enter my '
        read(*,*) my
        goto 94
    end if

    else if (nbeads.lt.1) then
        write(6,*) 'You are not funny.'
        stop

    else if(nbeads.eq.1) then

997  write(6,*) 'Enter the initial setup of liquid molecules;'
        write(6,*) ' only fcc lattice structure is allowed;'
        write(6,*) ' enter [0] for special crystal ordering'
        write(6,*) '      [1] for regular crystal ordering'
        read(5,*) ilat
        if(ilat.ne.0 .and. ilat.ne.1) then
            write(6,*) 'No. ',ilat,' is not a choice.'
            write(6,*) 'Try again.'
            goto 997
        end if
    end if

    if (ilat.eq.1) then
        write(6,*) 'Desired ordering of fluid lattice'
        write(6,*) 'fcc lattice => completely filled crystal!'
        write (6,*) 'Number of fluid layers =?'
        read(5,*) mz
        write (6,*) 'Scaling factor, f_z, for wall separation =?'
        read(5,*) fz
        write(6,*) 'No. of molecule cells in x & y direction: mx, my?'
        read(5,*) mx, my
97  continue
        if (mod(mx,2).ne. 0) then
            write(*,*) 'mx must be even. Try again, please.'
            write(*,*) 'Enter mx '
            read(*,*) mx
            goto 97
        end if
98  continue
        if (mod(my,2).ne. 0) then
            write(*,*) 'my must be even. Try again, please.'
            write(*,*) 'Enter my '
            read(*,*) my
            goto 98
        end if

    else if(ilat.eq.0) then
        write(6,*) 'Special ordering of fluid lattice!'
        write(6,*) 'fcc lattice => paritally filled crystal!'
        write(6,*) 'Enter fluid height, hz'
        read(5,*) hz
        write(6,*) 'Enter wall size: nxw, nyw'

```

```

write(6,*) 'i.e. number of wall layer in the x-, y-direction'
write(6,*) 'caution: be aware of the definition of nxw & nyw'
read(5,*) nxw, nyw
333 continue
if (mod(nxw,2).ne. 0) then
write(6,*) 'nxw must be even. Try again, please.'
write(6,*) 'Enter wall size: nxw '
read(5,*) nxw
goto 333
end if
334 continue
if (mod(nyw,2).ne. 0) then
write(6,*) 'nyw must be even. Try again, please.'
write(6,*) 'Enter wall size: nyw '
read(5,*) nyw
goto 334
end if
end if

write (6,*) 'Wall density?'
read(5,*) dens_w
write (6,*) 'monomer density =?'
read(5,*) dens

iwall = 1

c write(6,*) 'Are there walls [yes=1]?'
c read(5,*) iwall
c if(iwall.eq.1) then
c end if

write(6,*) 'Do you want to model a thermal wall?'
write(6,*) 'Your choices are as follows:'
write(6,*) 'Enter 0 for no; walls with stationay solid atoms'
write(6,*) ' 1 for yes; walls with thermally vibrating atoms'
335 continue
read(5,*) ithw
if (ithw .gt. 1) then
write(6,*) 'Incorrect input; value should be 0 or 1'
go to 335
endif

bond = 0.96
a_wall = (4./dens_w)**(1./3.)
a_nn = a_wall/sqrt(2.0)
box = vol**(1./3.)

ntypes = 3 + ithw*2

c.... For atomic fluid, the number of sites in a cell is 2. This is
c.... why mx originally must be even.
if (nbeads.eq.1) then
nsites = 2
mx = mx / 2
a_f = (4.0/dens)**(1./3.)
a_nn_f = a_f / sqrt(2.0)
else
nsites = nbeads
a_nn_f = bond

```

```

end if

write(6,*)
write(6,*) a_nn_f
write(6,*)

if(ilat.eq.1) then
  natom = mx*my*mz*nsites
  nmol = mx*my*mz
  fx = a_nn / (a_nn_f*sqrt(fz))
  fy = a_nn / (a_nn_f*sqrt(fz))

c....  if fluid cell length much shorter than wall cell length
c....  increase wall n?w.
  if (fx.lt.0.9) then
    nxw = float (mx * nsites) / fx + 1
    if (mod(nxw,2).ne. 0) nxw = nxw + 1
    fx = a_nn * nxw / (a_nn_f*2.*mx*sqrt(fz))
  else
    nxw = nsites * mx
  end if
  if (fy.lt.0.9) then
    nyw = float (my) / fy + 1
    if (mod(nyw,2).ne. 0) nyw = nyw + 1
    fy = a_nn*nyw / (a_nn_f*my*sqrt(fz))
  else
    nyw = my
  end if

c
  cellx = a_nn_f * xfp * float(nsites) / 2.0
c
  celly = a_nn_f * yfp
c
  cellz = fz*a_nn * zfp

c
  hx= a_nn *nxw * xfp / 2.0
c
  hy= a_nn*nyw * yfp

c....  Use a_nn instead of bond for layer spacing.
c
  hz= mz*fz*a_nn*zfp
c
  vol = hx*hy*hz

  dz = hz / float(mz)

  else if(ilat.eq.0) then

c....  This code is not intelligent, but ....
c
  hx= a_nn*nxw*xfp/2.0
c
  hy=a_nn*nyw*yfp

c....  Use a_nn instead of bond for layer spacing.
  vol = hx*hy*hz

```

```

    natom = dens * vol
    nmol = natom
end if

c    if(a_nn_f.gt.1.0) then
c      write(6,*) 'WARNING: a_nn_f is larger than wall a_nn.'
c    end if

c
c    dz_w = a_wall/sqrt(3.0)
c    dz_w = a_wall/2.0

dz_w = a_wall*zfp/sqrt(2.0)

expand = dz/dz_w

nwall=nxw*nyw*4
c
nbonds = nwall*ithw + nmol*(nbeads-1)
ntot = natom + nwall*(ithw+1)

dens_foo = natom / vol

write(6,*) 'a_nn = ', a_nn
write(6,*) 'nmol = ', nmol

hx2 = hx*hx
hy2 = hy*hy
hz2 = hz*hz

c.... separation distance between walls and outer limit of walls
zmax = hz + 2.0*(1.0+dz_w)

write(6,*) ' '
write(6,*) 'Expansion factor = ', expand
write(6,*) 'fluid layer spacing = ', dz
write(6,*) 'wall layer spacing = ', dz_w
write(6,*) 'Number of wall atoms = ', nwall
write(6,*) 'Number of fluid atoms = ', natom
write(6,*) 'wall density = ', dens_w
write(6,*) 'fluid density = ', dens
write(6,*) 'volume = ', vol
write(6,*) 'nxw = ', nxw
write(6,*) 'nyw = ', nyw
write(6,*) 'mx = ', mx
write(6,*) 'my = ', my
write(6,*) 'mz = ', mz
write(6,*) 'fx = ', fx
write(6,*) 'fy = ', fy
write(6,*) 'fz = ', fz
write(6,*) ' '

hxa = hx/2.0
hya = hy/2.0
hza = zmax/2.0
c.... Box is in LJ units
sigma = 1.
epsilon = 1.
write(6,*) ' '

```

```

if(iwall.eq.1) then
  write(6,*) 'hx = ', hx
  write(6,*) 'hy = ', hy
  write(6,*) 'hz = ', hz
else
  write(6,*) 'box = ', box
end if
write(6,*) ' '

if(natom.gt.nmax) then
  write(6,*) 'Number of atoms too large! num > nmax = ', nmax, '
  write(6,*) 'Please edit program and recompile.'
  stop
end if

```

c.... Output

```

nero = 0
i1 = 1
open(8,file='input.lammps',status='unknown')
write(8,*)
write(8,*)
write(8,*) ntot, ' atoms'
write(8,*) nbonds,' bonds'
write(8,*) nero, ' angles'
write(8,*) nero, ' dihedrals'
write(8,*) nero, ' impropers'
write(8,*)
write(8,*) ntypes,' atom types'
write(8,*) i1 , ' bond types'
write(8,*)
write(8,*) -hxa,hxa,' xlo xhi'
write(8,*) -hya,hya,' ylo yhi'
write(8,*) -hza,hza,' zlo zhi'
write(8,*)
write(8,602) 'Atoms'
write(8,*)
602 format(a5)

p0 = 0.0

if(ilat.eq.1) then
  call mkfluid(mx,my,mz,dz)
else if(ilat.eq.0) then
c
c randomly placing atoms has been replaced by fcc-limited
c call mkfluid_rand
c
  call mkfluid_fcc0(dens)
end if

do i=1,natom
  xc(i) = x0(i,1) * hx
  yc(i) = x0(i,2) * hy
  zc(i) = x0(i,3) * hz
end do

c.... OUTPUT
c.... atoms
c.... MY PERSONAL VERSION NEEDS 3 nero-s at end!

```

```

amass = 1.
itype = 1
chg = 0.0
do i=1,natom
  moltype = itype
  write(8,10) i,moltype,itype,chg,xc(i),yc(i),zc(i),
+      nero,nero,nero
end do
call flush(8)

c.... XMol output
open(2,file='input.xmol',status='unknown')
write(2,*)ntot
write(2,*)' '
do i = 1, natom
  write(2,'(a4,3f16.5)')'YR ', xc(i),yc(i),zc(i)
end do
call flush(2)

c.... Alchemy output
open(3,file='input.alc',status='unknown')
write(3,134) ntot,nbonds,nero
134 format(i5,1x,'ATOMS',1x,i5,1x,'BONDS',1x,i5,1x,'CHARGES')
do i = 1, natom
  write(3,'(i5,1x,a4,2x,3(f8.4,1x),2x,f8.4)')
1      i,'YR ', xc(i),yc(i),zc(i),p0
end do
call flush(3)

if(iwall.eq.1) call mkwall(nxw,nyw,a_wall,dz_w)

c.... Bonds to represent the thermal wall

if (ithw .eq. 1) then
  write(8,*)
  write(8,602) 'Bonds'
  write(8,*)

  k = 0
  itype = 1
c.... Bottom wall
  do i1=1,nwall/2
    i=natom + i1
    j=i+nwall/2
    k = k+1
    write (8,139) k,itype,i,j
  end do
c.... Top wall
  i0 = natom + nwall
  do i1=1,nwall/2
    i=i0 + i1
    j=i+nwall/2
    k = k+1
    write (8,139) k,itype,i,j
  end do
endif
139 format(4i6)

c.... Masses

```

```

write(8,*)
write(8,603) 'Masses'
write(8,*)
603 format(a6)
do i=1,ntypes
  write(8,12) i,z1
end do
12 format(i6,1x,f6.2)

c.... Bonds

if(nbeads.gt.1) then

c.... Alchemy Bonds
k=0
do i1=1,nmol
do i2=1,nbeads-1
  i=(i1-1)*nbeads + i2
  j=i+1
  k = k+1
  write (3,133) k,i,j
end do
end do
133 format(3(i5,1x),' SINGLE')
call flush(3)

write(8,*)
write(8,602) 'Bonds'
write(8,*)
k=0
do i1=1,nmol
do i2=1,nbeads-1
  i=(i1-1)*nbeads + i2
  j=i+1
  k = k+1
  write (8,13) k,itYPE,i,j
end do
end do
13 format(4i6)
call flush(8)
end if

c.... LJ coeff
c write(8,*)
c write(8,604) 'Nonbond Coeffs'
c write(8,*)
c 604 format(a14)
c do itype =1,ntypes
c do jtype=itype,ntypes
c write(8,*) itype,jtype,epsilon,sigma
c end do
c end do

close(8)

10 format(i6,1x,i5,1x,i2,1x,f6.2,3(1x,f9.4),3i6)

end

```

```

subroutine mkwall(nxw,nyw,a_wall,dz)
c
c.... This routine creates an fcc [111] or [001] lattice composed of
c.... "solid" atoms. The geometry is that of a Couette cell.
c.... Two walls, parallel to the x-y plane, confine a fluid with
c.... periodic BCs in the x and y directions. The fcc lattice is
c.... constructed as follows:
c.... ifcc=1 the [100] direction is along the positive x-axis
c.... ifcc=2 the [112bar] direction is along the positive x-axis
c.... ifcc=3 the [1bar10] direction is along the positive x-axis
c
c.... Parameters which determine the lattice:
c.... nxw,nyw = # of wall particle layers in the x and y-directions
c....
c.... The # of wall particles = nxw*nyw*4, since there are 2 layers
c.... of wall atoms per wall.
c....
c.... Finally, note that the positions of all the fluid particles lie
c.... within a -0.5 to 0.5 unit cell. The same holds true for the x and y
c.... degrees of freedom of the wall particles. However, the location
c.... of the wall particles in the z direction lie OUTSIDE the
c.... -0.5 to 0.5 unit cell.
c
parameter(npart=5000)
dimension y1(3),x0(npart,3)
c dimension tmpx(npart),tmpy(npart),tmpz(npart),vf(npart)
common/hmatrix/ hx,hy,hz,cellx,celly,cellz,fx,fy
common/numbers/ natom,nbeads,nsites,ifcc,ithw
c
c.... Compute particle numbers
c
molsw=nxw*nyw*4
if (molsw.gt.npart) then
write(*,*) "Error: too many wall atoms in subroutine mkwall"
stop
endif
molw=molsw/2
molw4=molsw/4
c
c.... Define various variables

y1(1)=0.0
y1(2)=1.0
y1(3)=2.0
c
110 continue
go to (111,112,113), ifcc
write(*,*) 'error: ifcc must be less than 4.'
go to 110
111 rfp = 1.0
go to 115
112 rfp = 2.0/3.0
go to 115
113 rfp = 2.0/3.0
go to 115

115 continue

```

c.... Set-up fluid lattice starting with lower left corner.  
 c.... Lattice goes ABCABC.. along z-axis.  
 c.... Now set-up wall lattice.

```

fx_tmp=1.0/float(nxw)
fy_tmp=1.0/float(nyw)
fz_tmp=dz/hz
c1=-0.5+.250*fy_tmp
c2=-0.5+0.50*fx_tmp

```

c.... zspace is the spacing between the (111) or (001) (z)layers.  
 c.... wlayr is the spacing between the simulation cell and the first wall layer.  
 c.... The choice with 1/hz is 1 sigma from the sim cell.

```

zspace=fz_tmp
wlayr=0.50*(1.0+fz_tmp)
c wlayr=0.50 + 1.0/hz

```

```

ii=0
c.... Loop over layers in z-direction
do k=1,2
c.... Loop over layers in y-direction
do i=1,nyw
c.... Loop over layers in x-direction
do j=1,nxw
mm=2-mod(j,2)
jshift=(j+1)/2
ii=ii+1
x0(ii,2)=c1+(float(i-1)+0.5*y1(mm))*fy_tmp
c
x0(ii,1)=c2+(2.*float(jshift-1)+y1(mm)+
+ rfp*y1(k))*fx_tmp

x0(ii,3)=-wlayr+float(k-2)*zspace

x0(ii+molw,2)=x0(ii,2)
c
x0(ii+molw,1)=c2+(2.*float(jshift-1)+y1(mm)+
+ rfp*y1(k))*fx_tmp

x0(ii+molw,3)= +wlayr + (k-1)*zspace
enddo
enddo
enddo

```

c.... Make sure particles are within primary simulation cell

```

do i=1,molsw
x0(i,1)=x0(i,1)-int(2*x0(i,1))
x0(i,2)=x0(i,2)-int(2*x0(i,2))
enddo

```

c.... Convert to LJ cell.

```

do i=1,molsw
x0(i,1) = x0(i,1)*hx
x0(i,2) = x0(i,2)*hy
x0(i,3) = x0(i,3)*hz
end do

```

c.... Lammmps OUTPUT

```

chg = 0.0

if (ithw .eq. 0) then
  itype = 2
  moltype = itype
  do i=1,molw
    j=natom+i
    write (8,10) j,moltype,itype,chg,x0(i,1),x0(i,2),x0(i,3),
1      nero,nero,nero
  end do

  itype = 3
  moltype = itype
  do i=molw+1,molsw
    j=natom+i
    write (8,10) j,moltype,itype,chg,x0(i,1),x0(i,2),x0(i,3),
1      nero,nero,nero
  end do

else
  itype = 2
  moltype = itype
  do i=1,molw
    j=natom+i
    write (8,10) j,moltype,itype,chg,x0(i,1),x0(i,2),x0(i,3),
1      nero,nero,nero
  end do

  itype = 3
  moltype = itype
  jstart = natom + molw
  do i=1,molw
    j=jstart+i
    write (8,10) j,moltype,itype,chg,x0(i,1),x0(i,2),x0(i,3),
1      nero,nero,nero
  end do

  itype = 4
  moltype = itype
  jstart = natom + molw
  do i=molw+1,molsw
    j=jstart+i
    write (8,10) j,moltype,itype,chg,x0(i,1),x0(i,2),x0(i,3),
1      nero,nero,nero
  end do

  itype = 5
  moltype = itype
  jstart = natom + molsw
  do i=molw+1,molsw
    j=jstart+i
    write (8,10) j,moltype,itype,chg,x0(i,1),x0(i,2),x0(i,3),
1      nero,nero,nero
  end do
endif

10 format(i6,1x,i5,1x,i2,1x,f6.2,3(1x,f9.4),3i6)

```

```

call flush(8)

c.... XMol output:
do i=1,molw
  write(2,150)'XG',x0(i,1),x0(i,2),x0(i,3)
end do
do i=molw+1,molsw
  write(2,150)'XB',x0(i,1),x0(i,2),x0(i,3)
end do
150 format(a2,2x,3f16.5)
call flush(2)
c.... Alchemy output:
do i=1,molw
  j = i+ natom
  write(3,151)j,'XG ',x0(i,1),x0(i,2),x0(i,3),p0
end do
do i=molw+1,molsw
  j = i+ natom
  write(3,151)j,'XB ',x0(i,1),x0(i,2),x0(i,3),p0
end do
151 format(i5,1x,a4,2x,3(f8.4,1x),2x,f8.4)

return
end

subroutine mkfluid(mx,my,mz,dz)
c
c.... This routine creates an fcc lattice.
c.... for [111] lattice goes ABCABC.. along z-axis.
c.... for [001] lattice goes ABABAB.. along z-axis
c.... Parameters which determine the lattice:
c.... mx,my,mz = # of molecular particle layers in the x,y,z-directions
c.... Lattice structure in xy plane: x direction is 11-2
c.... The simple cell for single atoms looks like this
c....   O * x 0
c....   x O *
c....   O * x 0
c.... For N=4, the lattice looks like this, where the bonds are missing.
c....   x  x   x  x
c....   x O * x O *   x O * x O *
c....   O * 0 * 0 O * 0 * 0
c....
c....   x  x   x  x
c....   x O * x O *   x O * x O *
c....   O * 0 * 0 O * 0 * 0

c....
c.... Finally, note that the positions of all the fluid particles lie
c.... within a -0.5 to 0.5 unit cell.
c
parameter(nmax=100000)
c dimension x1(3),y1(3),z1(3)
dimension x1(3),y1(3)
common/hmatrix/ hx,hy,hz,cellx,celly,cellz,fx,fy
common/numbers/ natom,nbeads,nsites,ifcc,ithw
common/fluid/ x0(nmax,3)

110 continue
go to (111,112,113), ifcc

```

```

write(*,*) 'error: ifcc must be less than 4.'
stop

111  xfp = sqrt(2.0)
     yfp = sqrt(2.0)
     zfp = sqrt(2.0) / 2.0
     rfp = 1.0
     ifp = 2
     go to 115
112  xfp = sqrt(3.0)
     yfp = 1.0
     zfp = sqrt(6.0) / 3.0
     rfp = 2.0/3.0
     ifp = 3
     go to 115
113  xfp = 1.0
     yfp = sqrt(3.0)
     zfp = sqrt(6.0) / 3.0
     rfp = 2.0/3.0
     ifp = 3
     go to 115

115 continue

c.... The metric for the unit cell.
     sx=cellx/hx
     sy=celly/hy
     sz=1.0/float(mz)

c.... Define various variables
c.... shift factors for different layers of ABC stacking
     x1(1)=0.0
     x1(2)=1.0/float(ifp) * sx
     x1(3)=2.0/float(ifp) * sx
     y1(1)=0.0
     y1(2)=0.5 * sy
     y1(3)=0.0

c presently do not need
c   z1(1)=0.0
c   z1(2)=1.0/3.0 * sz
c   z1(3)=2.0/3.0 * sz

c.... Shift in unit cell of cell origin due to factors fx and fy
c.... and shift 1/2 a layer thickness (sz/3) from the wall atoms.
     dx = fx*sx
     dy = fy*sy
     wlayer=-0.5 + 0.5*sz

c.... kk defines the stacking corresponding to ABC or ABAB.
     ii=0
c.... Loop over layers in z-direction
     do k=1,mz
c.... Loop over layers in y-direction
     do i=1,my
c.... Loop over layers in x-direction
     do j=1,mx
     do jj=1,nsites

```

```

ii=ii+1
kk = mod(k-1,ifp)+1
xj = float(jj-1)/float(nsites)
x0(ii,1) = xj*sx + rfp*x1(kk) + dx*(j-1) - 0.5
*       + 0.5*sx/float(nsites)

if (nbeads.eq.1) then
  if(kk.eq.ifp) then
    yi = mod(jj,2)/2.0*sy
  else
    yi = mod(jj-1,2)/2.0*sy
  end if
  x0(ii,2) = yi + y1(kk) + dy*(i-1) - 0.5
*       + 0.25*sy
else
  x0(ii,2) = mod(jj-1,2)/2.0*sy + y1(kk)
*       + dy*(i-1) - 0.5 + 0.25*sy
end if
x0(ii,3) = (k-1)*sz + wlayer
enddo
enddo
enddo
enddo

```

c.... Make sure particles are within primary simulation cell

```

do i=1,natom
  x0(i,1)=x0(i,1)-int(2*x0(i,1))
  x0(i,2)=x0(i,2)-int(2*x0(i,2))
  x0(i,3)=x0(i,3)-int(2*x0(i,3))
enddo

```

```

return
end

```

c

c This subroutine has been replaced by mkfluid\_fcc0

```

subroutine mkfluid_rand

```

c....

c.... Present version only works for nbeads=1

```

parameter(nmax=100000)
c dimension x1(3),y1(3),z1(3)
common/hmatrix/ hx,hy,hz,cellx,celly,cellz,fx,fy
common/hmatrix2/ hx2,hy2,hz2
common/numbers/ natom,nbeads,nsites,ifcc,ithw
common/fluid/ x0(nmax,3)

```

c.... rc2 is the minimum square separation allowed.

```

i = 0
p0 = 0.0
p5 = 0.5
rc2 = 0.9
zh=hz-0.3
zh2=zh*zh

```

```

iseed = 12345

```

```

r = drand(iseed)

```

```

do i=1,natom
  jcount = 0
102  continue
c.... Can't find appropriate position.
      jcount = jcount+1
      if(jcount.gt.500000) then
        write(6,*) 'Having difficulties placing particles.'
        write(6,*) i,' jcount=500000'
        jcount = 0
      end if

c.... get random position in unit cell [-.5,+.5]^3
      rd = drand(0)
      x = rd - p5
      rd1 = drand(0)
      y = rd1 - p5
      rd2 = drand(0)
      z = rd2 - p5

c
c   x = (rand(0) - p5)
c   y = (rand(0) - p5)
c   z = (rand(0) - p5)
c   print *, x,y,z

      x = x - anint(x)
      y = y - anint(y)
      z = z - anint(z)
c.... Check for overlap.
      do j = 1,i-1
        xd = x0(j,1) - x
        yd = x0(j,2) - y
        zd = x0(j,3) - z
        xd = xd - int(2*xd)
        yd = yd - int(2*yd)
        zd = zd - int(2*zd)
        rd2 = xd * xd * hx2 + yd * yd * hy2 + zd * zd * hz2
        if(rd2.le.rc2) goto 102
      end do

c.... We have a winner!
      x0(i,1) = x
      x0(i,2) = y
      x0(i,3) = z
    end do

c.... Make sure particles are within primary simulation cell
      do i=1,natom
        x0(i,1)=x0(i,1)-int(2*x0(i,1))
        x0(i,2)=x0(i,2)-int(2*x0(i,2))
        x0(i,3)=x0(i,3)-int(2*x0(i,3))
      enddo

      return
    end

subroutine mkfluid_fcc0(dens)
c

```

```

c.... This routine creates an fcc [001] lattice.
c.... Parameters which determine the lattice:
c....  nxf,nyf = # of fluid particle layers in the x and y-directions
c....
c....  The # of fluid particles = nxf*nyf*nyz,
c....
c.... Finally, note that the positions of all the fluid particles lie
c.... within a -0.5 to 0.5 unit cell.
c
  parameter(z1=1.0,nmax=100000)
  common/hmatrix/  hx,hy,hz,cellx,celly,cellz,fx,fy
  common/hmatrix2/ hx2,hy2,hz2
  common/numbers/  natom,nbeads,nsites,ifcc,ithw
  common/fluid/   x0(nmax,3)

  dimension y1(3)
c  dimension tmpx(nmax),tmpy(nmax),tmpz(nmax),vf(nmax)

110 continue
  go to (111,112,113), ifcc
  write(*,*) 'error: ifcc must be less than 4.'
  stop

111  xfp = sqrt(2.0)
  yfp = sqrt(2.0)
  zfp = sqrt(2.0) / 2.0
  rfp = 1.0
  ifp = 2
  go to 115

112  xfp = sqrt(3.0)
  yfp = 1.0
  zfp = sqrt(6.0) / 3.0
  rfp = 2.0/3.0
  ifp = 3
  go to 115

113  xfp = 1.0
  yfp = sqrt(3.0)
  zfp = sqrt(6.0) / 3.0
  rfp = 2.0/3.0
  ifp = 3
  go to 115

115 continue

c.... Define various variables
  y1(1)=0.0
  y1(2)=1.0
  y1(3)=2.0
c
  hz0=hz
c
  a_f1=(4.0/dens)**(1./3.)
c
c*** (ccw) did not imply yet but will consider later
c
c  scale0=1.0
c  write(6,*) 'Scaling factor in term of fluid fcc cubic edge:'
c  read(*,*) scale0
c  a_f1=scale0*a_f1

```

```

c
do nn=1,30
c
  nxtmp=2*int(hx/a_f1*sqrt(2.0)/xfp)
  nytmp=int(hy/a_f1*sqrt(2.0)/yfp)
  nztmp=int(hz0/a_f1*sqrt(2.0)/zfp)

  ntott=nxtmp*nytmp*nztmp
  if (ntott.ge.natom) go to 99
  a_f1=0.99*a_f1
enddo
write(*,*) 'nn>30, fluid spacing is too close; stop!'
stop

99 continue
a_ff=a_f1
nxf=nxtmp
nyf=nytmp
nzf=nztmp
write(6,*) 'a_f1= ',a_f1,' nxf= ',nxf,' nyf= ',nyf,
+         ' nzf= ',nzf

c.... Set-up fluid lattice starting with lower left corner.
c.... Lattice goes ABCABC.. along z-axis.
c.... Now set-up wall lattice.

fx_tmp=1.0/float(nxf)
fy_tmp=1.0/float(nyf)
fz_tmp=1.0/float(nzf)

c1=-0.5+.250*fy_tmp
c2=-0.5+0.50*fx_tmp

c.... zspace is the spacing between the (001) (z)layers.
c.... wlayr is the -position of the first layer
zspace=fz_tmp
wlayr=0.50*(1.0-fz_tmp)

ii=0
c.... Loop over layers in z-direction
do k=1,nzf
c.... Loop over layers in y-direction
do i=1,nyf
c.... Loop over layers in x-direction
do j=1,nxf
  mm=2-mod(j,2)
  jshift=(j+1)/2
c
  kk = mod(k-1,ifp)+1

  ii=ii+1
  x0(ii,2)=c1+(float(i-1)+0.5*y1(mm))*fy_tmp

  x0(ii,1)=c2+(2.*float(jshift-1)+y1(mm)+
+         rfp*y1(kk))*fx_tmp

  x0(ii,3)=-wlayr+float(k-1)*zspace
  if (ii.ge.natom) goto 999

```

```
    enddo  
  enddo  
enddo
```

```
999 continue
```

```
c.... Make sure particles are within primary simulation cell
```

```
do i=1,natom  
  x0(i,1)=x0(i,1)-int(2*x0(i,1))  
  x0(i,2)=x0(i,2)-int(2*x0(i,2))  
  x0(i,3)=x0(i,3)-int(2*x0(i,3))  
enddo
```

```
return  
end
```

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