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New indirect method for calculation of flow forces in molecular dynamics simulation

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ABSTRACT

A new method for calculation of fluid flow forces in molecular dynamics (MD) simulations is proposed herein. We call this method Molecular Momentum Balance method. This method together with two other methods reported in literature are used in an in-house, parallel MD code to calculate drag force exerted on a carbon nanotube in a uniform flow of liquid argon, as well as skin wall friction in argon channel flow. The two methods used as a benchmark are a method based on direct summation of forces exerted by fluid molecules, called the Direct Method herein, and a method based on the flow momentum balance obtained from the mean velocity profile, called the momentum balance method herein. Carbon nanotube is modeled as a rigid cylinder, and the channel walls are modeled with two layers of carbon atoms. All the interactions are modeled using Lennard-Jones potential function. In the case of carbon nanotube, results indicate that at best, the momentum balance method generates 20% error compared to the drag force calculated by the direct method. This error does not noticeably decrease by increasing the number of bins used for capturing the mean velocity profile. In contrast to this, the present method, i.e. the molecular momentum balance generates a very small error compared to the results from the direct method. This error can be reduced to less than 1% by increasing the time period in which data are averaged. Based on this experience, the present method was applied to calculate skin friction drag in two channel flows, i.e. a channel with spring-mounted carbon wall molecules, and a channel with rigid carbon wall molecules. The results were within 0.1% of those from the direct method. This confirms that the new method works properly to predict flow forces in different MD simulations.

1. Introduction

In recent years, the study of fluid flow in nanoscales has been a subject of interest. Due to the lack of experiment in nanoscales, the role of numerical methods has been significant [1]. At length scales less than ten molecular diameters continuum theory is no longer valid in both gas and liquid flows [2]. Therefore numerical methods for the simulation of continuum fluid flow cannot be used in this regime. To study the behavior of fluid flow in the atomistic level, the powerful method of MD simulation can be used. This method is suitable for the simulation of problems in the length scale of 100 nm or less [3].

Prediction of flow forces is of significant importance in MD simulations of fluid flow. Vergeles et al. [4] studied translational and rotational motions of a sphere in a viscous liquid using MD simulation. In their study, a summation of fluid forces exerted on the body at molecular level was directly performed to obtain the fluid forces; we call this, "direct method". It was reported that the drag and torque on a sphere in an effectively unbounded fluid are found to be in agreement with continuum hydrodynamics. Walther et al. [5] calculated drag forces for carbon nanotubes (CNTs) in water flow. They also showed that drag coefficients calculated by direct method are in reasonable agreement with those obtained from macroscopic Stokes-Oseen solution. In a more detailed and systematic study, Tang and Advani [1] calculated drag coefficient of a CNT in liquid argon flow using Non-Equilibrium MD (NEMD) simulation. Here again, direct summation of molecular forces was used to evaluate the drag forces and its coefficients on two different sizes of CNTs in a wide range of flow velocities from 15 to 320 m/s. This study showed that at low speed flows, drag coefficients obtained from MD simulations are larger than those obtained from finite element analysis and empirical equations. Ziarani and Mohamad [6] used a different method called "momentum balance method" to compute the fluid forces. In this method, lift and drag forces are calculated from the change of momentum, which is evaluated from the profile of mean flow velocity at each section. In their work, flow over two molecular cylinders in a side by side arrangement was simulated using two-dimensional NEMD simulation to validate the method. They found that the momentum balance method generates an error of about 25% compared to the direct method.

In all of the above studies lift and drag forces are evaluated using two different methods, either direct summation of molecular forces or momentum balance method. The reported difference between results of

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two methods is 25 to 30%. In these studies, no details are reported on how the velocity profile is measured or how the integral form of conservation of momentum is applied in MD simulations.

The objective of present work is to study different methods of force calculation in MD simulations. The method of momentum balance will be investigated in details and will be compared with the direct method. In addition, a new molecular method originated from continuum approach will be presented for the prediction of fluid forces in this paper, and its results will be compared with results of the other two methods.

2. MD simulation

In the current study, all variables and results will be expressed in reduced MD units, in which all variables are non-dimensionalized by the reference variables of molecular mass (m), diameter of liquid argon (σ), and strength of interaction for Lennard-Jones Potential (ε). Reference units for argon are given in Table 1. Time, force, and velocity variables are defined based on reference variables and for argon their units are given in Table 2.

All of the atoms interact according to Lennard-Jones (LJ) 12-6 potential function but with different parameters for argon–argon and carbon–argon. Interaction forces between argon–argon and carbon–argon atoms are computed using the parameters given in Table 3.

A cut-off distance of $r_c = 2.5$ is used for both interactions. The neighbor list method is also used to calculate interactions between atoms. Equation of motion is integrated using a Verlet scheme with a time step of $\Delta t = 0.001$ which is equal to 2.15×10^{-15} s. With these assumptions, an in-house, parallel MD code is developed in which, atom decomposition approach is used to reduce computational time. In all of the cases, MD simulation is performed for 8×10^5 time steps corresponding to 1.72 ns.

Two cases will be studied in this paper, Argon flow over a CNT, and argon flow within a channel. Calculation of drag force of a CNT is studied first and based on the results, a new method is proposed for this purpose. Having shown that the new method works very well in CNT case, it was then applied to calculate skin friction drag in the channel flow.

3. Carbon nanotube in uniform flow

As shown in Fig. 1, the case of nanotube consists of two types of atoms; argon atoms as fluids, and carbon atoms as the wall of CNT. Domain of simulation is a box with periodic boundary condition in all directions. Since different domain sizes will be considered here, a base domain is defined first with dimensions of $50 \times 60 \times 6.26$ in height (z-direction), length (y-direction), and width (x-direction), respectively. Sizes of other domains are referenced to this base domain. Note that widths of domains are always equal to the length of nanotube that is 6.26. A single walled (12, 0) CNT with the diameter of 2.76 is fixed in the middle of the geometry with an offset of $0.1L_y$ (6 for the base domain) from the center of the geometry to the inlet. The nanotube is modeled as a fixed body with rigid structure such that carbon atoms do not move relative to their initial positions.

Table 1
Reference units for argon.

Quantity	Symbol	Value
Length	σ	3.40×10^{-10}(m)
Mass	m	6.625×10^{-26}(kg)
Energy	ε	1.657×10^{-21}(J)

Table 2
Other units for argon.

Quantity	Symbol	Value
Time	$\tau \equiv \sigma(m\varepsilon^{-1})^{1/2}$	2.15×10^{-12}(s)
Force	$F \equiv \varepsilon\sigma^{-1}$	4.873×10^{-12}(N)
Velocity	$U \equiv \sigma\tau^{-1}$	1.58×10^{2}(m·s^{-1})

3.1. Initial setup and driving the flow

Liquid argon atoms with a density of 0.8 and total number of 14,964 are initially distributed in a lattice form of FCC in the base domain. Initial thermal velocities of atoms are assigned according to their initial temperature of 95 K. Velocity components of atoms are determined based on Maxwell–Boltzmann distribution that results in a zero total flow velocity. Initial mean flow then is generated by adding a velocity of $U_0 = 1.0$ in y direction to all argon atoms. To maintain flow, velocities of atoms located in the first $0.03L_y$ (1.8 for base domain) of the inlet region are reset to 1.0 every 50 time steps. Resetting or rescaling of velocity is applied by setting the initial random thermal velocity of the atoms in the inlet region and then adding U_0 to their velocities in y direction. This technique also removes excess heat from the system [7] and therefore, there is no need to use thermostat or other techniques.

3.2. Results

Before investigating methods for drag calculation, the present MD code was verified by solving the case of Tang and Advani [1]. In their work, the drag force exerted by uniform liquid argon flow on CNT (12, 0) was calculated for different domain sizes to investigate the effect of domain size on the drag force. Table 4 defines the domains used in Tang and Advani's study.

To evaluate the drag force of a nanotube, in our study, MD simulation is performed for a time of t_{eq} to reach equilibrium, and then is continued to a desired time of t_f to get enough data to extract flow forces on nanotube and other macroscopic properties. To detect equilibrium, other researches monitor either values of energy and pressure [8], or positional disorder and velocity distribution of atoms [9] with respect to time. In the present study, change of the kinetic energy with respect to time is monitored in the solution domain to detect the equilibrium state. The geometries defined in Table 4 are used to perform equilibrium state in MD simulations. In all cases equilibrium was reached after time durations ranging from 100 to 200 time units. Therefore, to assure equilibrium, t_{eq} of 200 is adopted for all of the simulations in this work. After t of 200, solution is continued up to 800 time units in all of the cases.

3.2.1. Direct method and code verification

In MD simulations, flow forces are calculated directly from the summation of forces exerted on the solid atoms by fluid atoms [1–5]. Instantaneous forces exerted on the nanotube in three directions of x, y and z fluctuate around their mean values. Mean value of forces are obtained from the following formulation, which is an average of the instantaneous forces over a period of time after equilibrium.

$$F_{ave} = \frac{1}{N_{t_{eq}-t_f}} \sum_{t_{eq}}^{t_f} F(t)_{inst} \tag{1}$$

Table 3
LJ potential parameters.

	Argon–Argon	Carbon–argon
ε	1.6567×10^{-21} (J)	1.9646×10^{-21} (J)
σ	3.4×10^{-10} (m)	3.573×10^{-10} (m)