Parameterizing the Morse potential for coarse-grained modeling of blood plasma

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Abstract

Multiscale simulations of fluids such as blood represent a major computational challenge of coupling the disparate spatiotemporal scales between molecular and macroscopic transport phenomena characterizing such complex fluids. In this paper, a coarse-grained (CG) particle model is developed for simulating blood flow by modifying the Morse potential, traditionally used in Molecular Dynamics for modeling vibrating structures. The modified Morse potential is parameterized with effective mass scales for reproducing blood viscous flow properties, including density, pressure, viscosity, compressibility and characteristic flow dynamics of human blood plasma fluid. The parameterization follows a standard inverse-problem approach in which the optimal micro parameters are systematically searched, by gradually decoupling loosely correlated parameter spaces, to match the macro physical quantities of viscous blood flow. The predictions of this particle based multiscale model compare favorably to classic viscous flow solutions such as Counter-Poiseuille and Couette flows. It demonstrates that such coarse grained particle model can be applied to replicate the dynamics of viscous blood flow, with the advantage of bridging the gap between macroscopic flow scales and the cellular scales characterizing blood flow that continuum based models fail to handle adequately.

1. Introduction

Viscous blood flow dynamics play a major role in cardiovascular devices (CVS) design process which in recent years relies more heavily on numerical simulation [1,2]. While the advent of these devices has provided life-saving solutions to millions of patients in the United States [3,4], thromboembolism remains an impediment in which shear induced platelet activation stimulates blood clotting [5–7]. To reduce the thrombogenic risk potential of the devices, efficient numerical simulations of blood flow need to be able to model not just the flow dynamics but processes pertinent to flow induced blood clotting. Computational fluid dynamics (CFD) is a well-established and universal continuum approach to study complex fluid flows. However, CFD simulations, while able to capture the overall flow mechanisms, are too coarse to model the finer features of blood particulate flow and fully describe the interactions of key players in blood coagulation such as platelets and other cells those may involve [8,9]. To address the limits of continuum approaches [10,11], dissipative particle dynamics (DPD) approach is introduced [12] to model heterogeneous fluids and biophysical details that are difficult to achieve using continuum approaches because the molecular effects, e.g., adhesion and aggregation bonds of blood clotting occur at the nano to micro scales. The coupling of the disparate spatial and time scales inspires multiscale simulation studies using...
approaches which depart from the continuum approaches [13–15]. A potential approach for such studies presented here is by coarse graining the atomistic based molecular dynamics (MD) to tradeoff between physical details and modeling feasibility.

In the past two to three decades, considerable efforts have been devoted to developing coarse-grained (CG) molecular models for studying polymers, bio membranes, surfactants and hemodynamics [16–24]. These CG models enable to focus on the particular scales of interactions by averaging the less essential degrees of freedom, resulting in a reduction of redundant computational loads. The selection of the degrees of freedom for coarse graining depends on the phenomena the simulation is trying to achieve. Therefore, some CG models encapsulate whole molecules while others treat several molecules as one effective CG particle. For example, one CG particle represents one water molecule in [16,18,20,25], or three water molecules in [23,24], or four in [26,27], or even five in [22], according to the simulation scales that best represent the phenomenon the simulation is trying to achieve. These CG models, while losing some resolution of the physical properties, enable us to consider larger systems within reasonable computational costs. Typically, the target properties include the thermodynamic properties, e.g., enthalpy of vaporization, free energy of solvation and interfacial tension, and statistical properties, e.g., radial distribution function and mean square displacement.

Developing a reliable CG model is challenging, in particular the effective force field with properly fitting parameters. Characteristically, a CG model simplifies the molecular description by smearing the interacting complexes, as save the computational cost of resolving the intricate details of physical properties. Deriving the effective potential analytically from statistical mechanics or other lower order principles may become limited to few simple cases [24]. A viable alternative for defining force field potential functions is to employ some simple and empirical models with a finite precision. Lennard–Jones (UJ) potential is the most popular pairwise non-bonded interaction model for simple applications, with limited accuracy. However, for, e.g., the case of complex viscous fluids, it offers only limited predictive capabilities [15]. Morse potential may fill the void in the “model space” although in its original form it is also limited. In 1929, physicist P.M. Morse developed the potential to describe chemical bond formation and dissociation [28]. In 2003, a Morse-like potential was adapted and proven capable of reproducing phase transitions and liquid–vapor coexistence curves of real fluids [17]. In 2010, it was parameterized for CG modeling of water and the n-alkanes and achieved a good agreement of various properties, including the enthalpy of vaporization, bulk densities, interfacial tensions, free energies of transfer, diffusion coefficients and isothermal compressibility [26].

In the current work we are extending the Morse potential approach presented in [26] to a CG model which includes a modification of the Morse potential, in order to simulate the flow of a blood plasma fluid. The key contributions of our work include parameterizing the model under multiple scales for fitting commonly used hemodynamic properties: density, pressure, isothermal compressibility and viscosity. Our model also reproduces the Counter-Poiseuille and Couette flows in agreement with these analytical benchmark solutions.

2. All-particle model and simulation

2.1. All-particle model

We model the blood plasma fluid by using CG particles, each of which lumps the aggregate effect of an ensemble of molecules. The total mass $M_{CG}$ of each CG particle is the sum of the masses of these molecules, measured in atomic mass unit (amu), and the position of a CG particle is the center of mass of this ensemble. The average distance $\mu$ is measured as the mean-free-path of the CG particles:

$$\mu = \rho_p^{-1/3} = (M_{CG}/\rho_m)^{1/3} \quad (1)$$

where $\rho_p$ and $\rho_m$ are the mass and particle density respectively. Obviously, for a system with fixed number of molecules, a larger $\mu$ implies a larger coarse-graining level, i.e., each CG particle contains more molecules. The growth of $\mu$ with the exponential increase of $M_{CG}$ is shown in Fig. 1, showing the relationship between $M_{CG}$ and the graining level.

We use a single water molecule of 18.015 amu as the mass unit of a basic molecule since blood plasma, which constitutes 55% of blood fluid, consists mostly of water (92% by volume). The W4 model, developed recently [26] for coarse-graining water, lumps four water molecules of 72.062 amu into one effective CG particle. In adapting the model to blood plasma we had to coarsen further the W4 model to include approximately 40 to 400 water molecules. Specifically, we extend the W4 model by further increasing the CG levels: $M_{CG} = 72, 720$ and 7206 amu for blood plasma. However, the original form of the Morse potential previously applied for the W4 model fails to express the interactions of the coarser model we are considering. After carefully studying several alternatives, we introduce the following modified Morse potential:

$$U_{ij}(r) = \varepsilon \left[ \exp(\alpha(1 - r/R(\mu))) - 2\exp(\alpha(1 - r/R(\mu))/2) \right] \quad (2)$$

where $R(\mu) = a/(\mu - b) + c$, $U_{ij}(r)$ is a pairwise non-bonded potential energy and $r$ is the relative distance of a particle pair, $R(\mu)$ is the distance of minimum energy $\varepsilon$ and $\alpha$ is a parameter that measures the curvature of the potential around $R(\mu)$. It contains three positive parameters $a$, $b$ and $c$ in units of $\AA^2$, $A$ and $A$ respectively. Parameter $a$ is related to the surface tension of the CG particle. It specifies the deviation of our modified Morse potential Eq. (2) from the original Morse potential and it becomes 0 when our model reduces to the original. The parameters: $\varepsilon$, $\alpha$ and $R(\mu)$ in Eq. (2) are obtained
Fig. 1. The relationship of the average distances over mass scales: $M_{CG}$ (amu) vs. $\mu$ (Å) where x-axis is in logarithm scale of base 10.

<table>
<thead>
<tr>
<th>Table 1</th>
<th>Mechanical properties of blood plasma fluid.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Properties</td>
<td>Symbol</td>
</tr>
<tr>
<td>Mass density</td>
<td>$\rho_{m,0}$</td>
</tr>
<tr>
<td>Diastolic/systolic blood pressures</td>
<td>$P_0$</td>
</tr>
<tr>
<td>Isothermal compressibility [37]</td>
<td>$\kappa_{T,0}$</td>
</tr>
<tr>
<td>Shear viscosity [38]</td>
<td>$\eta_0$</td>
</tr>
</tbody>
</table>

through the conventional inverse problem approach, i.e., the parameters are adjusted so that the simulation output best matches published blood plasma properties (summarized in Table 1).

2.2. Simulation

All simulations were performed at 310 K with NVT ensemble [29], using the LAMMPS (Large-scale of Atomic/Molecular Massively Parallel Simulator) code [30] (21-Dec-2011 version). A cubic box with 27,000 CG particles and mass scales of 72, 720 and 7200 amu were tested. Specific side lengths with reference to the density were used together with periodic boundary conditions. The CG particles are treated as mathematical dots for which all internal rotational and vibrational degrees of freedom within each CG particle are smeared out. The Berendsen thermostat method [31], which is realized by coupling to external bath, is implemented for temperature control. The isothermal compressibility $\kappa_T$ is calculated using the finite difference expression [32] and is expressed as:

$$\kappa_T = -\frac{1}{V} \left( \frac{\partial V}{\partial p} \right)_T = \left( \frac{\partial \ln(\rho)}{\partial p} \right)_T \approx \left( \frac{\ln(\rho_2/\rho_1)}{p_2 - p_1} \right)_T \tag{3}$$

The shear viscosity $\eta$ is calculated using the Green–Kubo (GK) method [33,34]. In this method, $\eta$ is given by integral of an accurate time-correlation of the equilibrium fluctuations of the corresponding flux and is expressed as:

$$\eta = \frac{V}{3k_B T} \int_0^\infty \sum \langle P_{\alpha\beta}(0) P_{\alpha\beta}(t) \rangle dt \tag{4}$$

where $\alpha\beta \in \{xy, yz, xz\}$, $V$ is the volume of the system, $k_B$ is the Boltzmann constant and $T$ is the temperature. $P_{\alpha\beta}$ refers to off-diagonal component of the pressure tensor. The angle brackets around the summation refer to an average of a "sufficiently large" sample. Eq. (4) can be re-written in the form:

$$\eta = \lambda \int_0^\infty C_{\alpha\beta}(t) dt \tag{5}$$

where $C_{\alpha\beta}(t)$ is the stress tensor autocorrelation function and $\lambda$ is a constant. Parameter $\tau_v$ is the characteristic time and is used for determining the number of samples to control the error $E_v$ at below 5%.
Table 2
Impact of model parameters on target properties.

<table>
<thead>
<tr>
<th>Change of parameter</th>
<th>Target property</th>
<th>( P )</th>
<th>( \kappa_T )</th>
<th>( \eta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Increase ( \alpha )</td>
<td>(-)</td>
<td>(-)</td>
<td>(-)</td>
<td>(-)</td>
</tr>
<tr>
<td>Increase ( R )</td>
<td>(\uparrow)</td>
<td>(\downarrow)</td>
<td>(\uparrow)</td>
<td></td>
</tr>
<tr>
<td>Increase ( \varepsilon )</td>
<td>(\downarrow)</td>
<td>(\downarrow)</td>
<td>(\uparrow)</td>
<td></td>
</tr>
<tr>
<td>Increase ( \rho )</td>
<td>(\uparrow)</td>
<td>(\downarrow)</td>
<td>(\uparrow)</td>
<td></td>
</tr>
</tbody>
</table>

3. Parameterization

Determining the interacting potential of CG particles involves at least two steps: (1) constructing the mathematical structures of the modified Morse potential and (2) deciding the parameters in the formula. This second step is referred to as parameterization and is accomplished through numerical experiments, as described below.

3.1. Classical Morse potential

A series of numerical experiments on classical Morse potential allowed us to understand the dependencies of different target properties on various parameters, summarized in Table 2. We notice that a series of models with \( \alpha = 7 \sim 10 \) are capable of reproducing desired properties, in particular, \( \alpha = 10 \) allows a longer timestep for dynamic simulations. \( R \) greatly influences the pressure; both \( \kappa_T \) and \( \eta \) are closely related with \( \varepsilon \); and, if \( \varepsilon \) is larger than some threshold, GK autocorrelation will diverge, resulting in a non-fluid behavior. With these observations, we exhaustively search the parameter space for the optimal set of parameters. Particularly, for a given \( M_{CG} \), we decouple the parameters in individual stages:

Stage 1: Given \( \alpha \) and \( \varepsilon \), search \( R \) to approximate \( P_0 \), resulting in a series of isothermal–isobaric curves under equilibrium. This yields \( R = R(\alpha, \varepsilon) \).

Stage 2: Given \( \alpha \), compute \( \kappa_T \) and \( \eta \) under a series of \( \varepsilon \) and \( R(\alpha, \varepsilon) \), to find the optimal combination.

To measure the accuracy of the approximating parameters, we normalize \( \kappa_T \) and \( \eta \) by dividing them by their target values. Obviously, the normalized \( \kappa_T \) or \( \eta \) is expected to be “1” as its ideal value.

Using the 2-stage approach, Fig. 2 demonstrates that the classical Morse potential is parameterized well to express interactions of all CG particles at \( M_{CG} = 72.06 \) amu (W4). However, the 2-stage exhaustive search approach fails to parameterize the classical Morse potential for the CG level of \( M_{CG} = 720.62 \) amu. This is depicted in Fig. 3: when desired \( \eta \) is obtained, \( \kappa_T \) is still far from its target value. On the other hand, when we continue increasing \( \varepsilon \) for improving \( \kappa_T \), GK autocorrelation diverges, driving the system out of its liquid phase range. This demonstrates that the classical Morse potential is inadequate for expressing the interactions of the larger CG particles needed for simulating blood plasma fluid.

3.2. Modified Morse potential

To address the limitation of the classical Morse potential we introduce a form factor \( R \) as a function of average distance \( \mu \). Accordingly, we modify the exhaustive search approach described in Section 3.1 as follows:

Stage 1: Given \( \alpha \) and \( \varepsilon \), search \( R \) to approximate \( P_0 \), resulting in a series of isothermal–isobaric curves under equilibrium. This yields \( R = R(\alpha, \varepsilon) \).

Stage 2: Given \( \alpha \), compute \( \eta \) under a series of \( \varepsilon \) and \( R(\alpha, \varepsilon) \), to find the optimal combination \( (\alpha_c, \varepsilon_c, R_c) \) for approximating \( \eta_0 \).
Stage 3: Given \((\alpha_c, \varepsilon_c, R_c)\), the system is compressed in a certain range to get a series of \(\{\mu_i\}_{i=0}^n\). The compression ratio is no more than 5%. The distance \(\mu_0\) measures the average distance of the uncompressed system and \(R_c\) is associated with \(\mu_0\). For \(\{\mu_i\}_{i=1}^n, \{R_i\}_{i=1}^n\) is adjusted to obtain the desired pressure increment as calculated in Eq. (3). Lastly, the form \(R(\mu) = a/(\mu - b) + c\) is adopted by applying a non-linear least square fit of the data points \((\mu_i, R_i)\).

Using this 3-stage approach, the modified Morse potential can be conveniently parameterized to express interactions of CG particles at the range of \(M_{CG} = 720.62\) through 7206.20 amu effective mass scales. Figs. 5 and 7 depict the pressure variation when the system is compressed, where the ideal values are computed through Eq. (3) and the experimental values are obtained through simulations. The corresponding functions \(R(\mu)\) are present in Figs. 4 and 6 respectively. The parameters for all tested CG levels are present in Table 3. In the table, we can see that a more coarsening level would lose some resolution of physical properties than a less coarsening level. For example, experimenting with various \(M_{CG}\) values indicates that the viscosity cannot reach the desired value for \(M_{CG} = 720.62\) amu at normal pressure but the characteristic viscosity could be maintained at a higher pressure. Therefore, we selected the parameters in Table 3 to enable our fit to most of the physical characteristics including the viscosity and the pressure. Although the high level of coarsening does increase the inaccuracies of the physical properties, these inaccuracies are under control and we are able to consider larger systems without adding too much computational cost.

4. Analysis

We tested and analyzed the model and parameters under three effective mass scales 72, 720 and 7200 amu, for determining the transport coefficients through Green–Kubo autocorrelation. We show structural properties by using the radial distribution functions, and validate two classic viscous flows scenarios – representing the behavior of our CG model for blood plasma flow under various shear stress conditions: Counter-Poiseuille flow and Couette flow. The impact of the simulation box changes on the results including the pressure, viscosity, compressibility and RDF profile is negligible, as shown in Appendix A.
Table 3
Parameters of the modified Morse potential for various mass scales: \( M_{CG} \) (mass of an effective CG particle, amu), \( \mu \) (average distance, Å), \( \rho_m \) (mass density, g/cm\(^3\)), \( \rho_p \) (particle density, \(10^{-3}\) particles/A\(^3\)), \( \alpha \) (curvature control parameter, a number), \( \varepsilon \) (minimum energy, kcal/mol), \( R = a/(\mu - b) + c \) (equilibrium distance, Å), \( a \) (Å\(^2\)), \( b \) (Å), \( c \) (Å), \( r_{cut} \) (cut-off distance of potential, Å), \( P \) (pressure, bar), \( \kappa_T \) (isothermal compressibility, \(10^{-5}\) bar\(^{-1}\)), \( \eta \) (shear viscosity, mPa·s).

<table>
<thead>
<tr>
<th>( M_{CG} )</th>
<th>( \mu )</th>
<th>( \rho_m )</th>
<th>( \rho_p )</th>
<th>( \alpha )</th>
<th>( \varepsilon )</th>
<th>( R = a/(\mu - b) + c )</th>
<th>( r_{cut} )</th>
<th>( P )</th>
<th>( \kappa_T )</th>
<th>( \eta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>720.06 amu</td>
<td>4.85</td>
<td>8.7776</td>
<td>1.05</td>
<td>10</td>
<td>0.00</td>
<td>12</td>
<td>1.5</td>
<td>5.44</td>
<td>0.97</td>
<td></td>
</tr>
<tr>
<td>720.62 amu</td>
<td>10.44</td>
<td>0.8778</td>
<td>0.0878</td>
<td>1.6</td>
<td>2.64</td>
<td>22.70</td>
<td>27</td>
<td>18.4</td>
<td>4.90</td>
<td>0.57</td>
</tr>
</tbody>
</table>

Fig. 8. Auto Stress Correlation functions \( C_{\alpha\beta}(t) \) vs. time (ps).

Table 4
Characteristic time of different CG levels: \( M_{CG} \) (mass distance, Å), \( dt \) (timestep, fs) and \( \tau_v \) (characteristic time, ps).

<table>
<thead>
<tr>
<th>( M_{CG} )</th>
<th>( \mu )</th>
<th>( dt )</th>
<th>( \tau_v )</th>
</tr>
</thead>
<tbody>
<tr>
<td>720.06 amu</td>
<td>4.85</td>
<td>15</td>
<td>0.35</td>
</tr>
<tr>
<td>720.62 amu</td>
<td>10.44</td>
<td>50</td>
<td>2.25</td>
</tr>
<tr>
<td>720.20 amu</td>
<td>22.50</td>
<td>100</td>
<td>5.00</td>
</tr>
</tbody>
</table>

4.1. Green–Kubo autocorrelation
We calculate the GK autocorrelation in a system of 27 000 CG particles. In the simulation, the sample interval is \( \Delta t = 5 \) and the timestep \( dt = 15, 50 \) and 100 fs for \( M_{CG} = 72, 720, 7206 \) amu respectively. We test and select a proper correlation length long enough to capture the decaying behavior but not too long to add noise. Parameter \( \eta \) is the integral of correlation function as in Eq. (4) and is presented in Table 3. Fig. 8 shows a normalized autocorrelation function. Table 4 summarizes the characteristic time \( \tau_v \) of the model under various CG levels.

4.2. Radial distribution function
We calculate the Radial Distribution Functions (RDF) for a system of 27 000 CG particles to validate the structural properties of our model at various CG levels as shown in Fig. 9.

4.3. Counter-Poiseuille and Couette flows
We test our model and parameters of different CG levels to reproduce two typical viscous flows: the Counter-Poiseuille and Couette flows, and compare the simulation results with the analytical solutions.

The Counter-Poiseuille flow is tested with three effective mass scales: \( M_{CG} = 72, 720, 7206 \) amu respectively. Fig. 10 illustrates the simulation domain for the Counter-Poiseuille flow. This domain is divided into a left region and a right region in which two opposing forces are applied on all fluid particles with magnitudes 0.05 kcal/mol/A in \( y \)-direction. A system size of \( 40 \times 20 \times 20 \) CG particles with periodic boundary conditions is utilized. We have run the simulation for 200 000 simulation steps in total. After 50 000 simulation steps, we observe that the Counter-Poiseuille flow is fully developed as the velocity profile no longer changes with time. The velocity profiles of fully developed Counter-Poiseuille flows for three mass scales are shown in Fig. 12.

Additionally, we test our model to reproduce the Couette flow with the same effective mass scales, system size and the total number of simulation steps as above. Fig. 11 illustrates the simulation domain for the Couette flow. This domain

Fig. 9. Radial distribution functions of the Morse fluids.

Fig. 10. Schematic representation of the periodic Poiseuille flow.

Fig. 11. Schematic representation of the Couette flow.

is divided into three regions: lower wall region, flow region and upper wall region. We apply two opposing forces with velocity magnitude of $-3.5$, $-1.1$, and $0.35$ A/ps respectively on all the upper and lower wall CG particles. We impose the PBC along the $x$- and $z$-directions and use virtual wall particles reflection method at the inner layer of $y$-direction walls to achieve a characteristic no-slip boundary condition at the interface of the fluid and the wall [29,35]. Briefly, wall reflection is applied such that if a particle moves outside the wall on a certain timestep by a distance delta, the particle is dragged back by the same delta, and the sign of the corresponding component of its velocity is flipped [29,30]. After 10,000 simulation steps, we observe that the Couette flow is fully developed as the velocity profile no longer changes with time. The velocity profiles of fully developed Couette flows for three mass scales are shown in Fig. 13.

The velocity profiles of fully developed Counter-Poiseuille and Couette flows are compared with the analytical solutions for all cases in Figs. 12 and 13. The analytical solution of Counter-Poiseuille is described by [36]:

$$v_y(x) = \frac{\rho g_y}{2\eta} (xD - x^2)$$

Here, $v_y$ is the velocity distribution, $\eta$ is the dynamic viscosity, $\rho$ is the mass density, and $g_y$ is the force.

These comparisons in Figs. 12 and 13 show that the velocity profiles of fully developed Counter-Poiseuille and Couette flows almost overlap with expected analytical solutions. Additionally, we observe no density fluctuations across the flow domains. This demonstrates the validity of our methodology for imposing no-slip boundary conditions and obtaining the
characteristic velocity distribution in both Counter-Poiseuille flow and Couette flow benchmark solutions for a broad range of spatiotemporal scales.

5. Conclusions

We modified the classical Morse potential to express the interactions of coarse-grained all-particle hemodynamics. The key contributions include the introduction of the form factor $R(\mu)$ to the classical Morse potential, in order to enable it to cover spatiotemporal scales ranging from atomistic scales to nano scales and to adapt it to capture the hallmarks of viscous flows dynamics. This facilitates studying complex flow mechanics such as of human blood plasma whose force field is approximated for the first time by this modified form of the Morse potential. Through extensive numerical experimentation, we obtained the parameters for three CG levels by multiple-staged methods as to parameterize the classical and modified Morse potentials. We have further studied the accuracy of our model by analyzing its transport coefficients and structural properties and validated it by reproducing two benchmark viscous flows solutions: Counter-Poiseuille and Couette flows.

Future work includes further verification of our model and parameters with more complex biological fluids such as blood constituents suspended in plasma, flowing in three-dimensional vasculature in patient specific geometries. Analyzing such complex fluids pushes the limit of continuum based numerical approaches as it requires an efficient multiscale methodology and fast parameterization scheme. Our model and methodology provides the means to realize such simulations at an appropriate CG level.

Acknowledgements

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Fig. 14. Results and analyses of the same simulation box using three coarse graining levels.

<table>
<thead>
<tr>
<th>$M_{CG}$ = 72.06 amu</th>
<th>$M_{CG}$ = 720.62 amu</th>
<th>$M_{CG}$ = 7206.20 amu</th>
</tr>
</thead>
<tbody>
<tr>
<td>Illustration of coarse graining levels</td>
<td><img src="image1" alt="Image" /></td>
<td><img src="image2" alt="Image" /></td>
</tr>
<tr>
<td>Total particles</td>
<td>2,744,000</td>
<td>262,144</td>
</tr>
<tr>
<td>Compressibility</td>
<td>5.52</td>
<td>4.38</td>
</tr>
<tr>
<td>Viscosity</td>
<td>0.93</td>
<td>0.98</td>
</tr>
<tr>
<td>Radial Distribution Function (RDF)</td>
<td><img src="image4" alt="Image" /></td>
<td><img src="image5" alt="Image" /></td>
</tr>
<tr>
<td>Poiseuille flows velocity profiles (x-axis: velocity in Å/ps; y-axis: position in Å)</td>
<td><img src="image7" alt="Image" /></td>
<td><img src="image8" alt="Image" /></td>
</tr>
<tr>
<td>Couette flows velocity profiles (x-axis: velocity $v_y$ in Å/ps; y-axis: position in Å)</td>
<td><img src="image10" alt="Image" /></td>
<td><img src="image11" alt="Image" /></td>
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</table>
Fig. 15. Comparisons of physical properties using different simulation boxes for $M_{CC} = 72.06$ amu. Note: * target physical properties are presented in Table 1.

<table>
<thead>
<tr>
<th>Box dimensions ($A^3$)</th>
<th>$145 \times 145 \times 145$</th>
<th>$675 \times 675 \times 675$</th>
<th>Target values *</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total particles</td>
<td>27,000</td>
<td>2,744,000</td>
<td></td>
</tr>
<tr>
<td>Compressibility ($10^{-5} \cdot bar^{-1}$)</td>
<td>5.44</td>
<td>5.52</td>
<td>4.6</td>
</tr>
<tr>
<td>Viscosity ($mPa \cdot s$)</td>
<td>0.97</td>
<td>0.93</td>
<td>1.1 ~ 1.3</td>
</tr>
<tr>
<td>Pressure ($bar$)</td>
<td>1.5</td>
<td>1.1</td>
<td>1.12 / 1.17</td>
</tr>
</tbody>
</table>

RDF

Fig. 16. Comparisons of physical properties using different simulation boxes for $M_{CC} = 720.62$ amu. Note: * target physical properties are presented in Table 1.

<table>
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<th>$675 \times 675 \times 675$</th>
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<tr>
<td>Total particles</td>
<td>27,000</td>
<td>262,144</td>
<td></td>
</tr>
<tr>
<td>Compressibility ($10^{-5} \cdot bar^{-1}$)</td>
<td>4.66</td>
<td>4.38</td>
<td>4.6</td>
</tr>
<tr>
<td>Viscosity ($mPa \cdot s$)</td>
<td>0.96</td>
<td>0.98</td>
<td>1.1 ~ 1.3</td>
</tr>
<tr>
<td>Pressure ($bar$)</td>
<td>1.2</td>
<td>1.2</td>
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</tr>
</tbody>
</table>

RDF

Appendix A. Impact of the system dimensions on coarse graining results

We build the identical system of size $675 A \times 675 A \times 675 A$ for three coarse-graining approaches. We perform the analysis by using a Radial Distribution Functions (RDF) and then compute the flow properties for both Couette and Counter-Poiseuille flows (as illustrated in Figs. 9, 12 and 13).

Fig. 14 presents the results and analyses of the same simulation box using three different coarsening levels. These results demonstrate that the physical properties vary slightly at different coarsening levels but the characteristics of the viscous flows stay unchanged. Figs. 15 and 16 compare the results of different simulation boxes using the same coarsening level. These results demonstrate that the impact of the simulation box changes on the results including the pressure, viscosity, compressibility and RDF profile is negligible.
References


[28] P.M. Morse, Diatomic molecules according to the wave mechanics. II. Vibrational levels, Phys. Rev. 34 (1) (1929) 57–64.


