The Approach of using Molecular Dynamics for Nanofluid Simulations

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Abstract—**The approach of using molecular dynamics (MD) for mimicking the dynamics of nanoparticles dispersion in different fluids is increasing since last decade. This vast increment utilizes computational softwares to mimick distictive aspects of experimental conditions. The technique of MD further makes it easier for understanding conditions of physical and chemical interactions that exist in nanofluid system.**

However, this review explains the procedure and implication on how to simulate the nanofluid system using molecular dynamics. Further, it is made easier for the reader for applying the technique, by good software recommendations and step by step procedure are given for utilization of successful nanofluid simulations.

Keywords—Nanofluid; Molecular dynamics; Brownian; Diffusion; Dispersion.

I. INTRODUCTION

The word nanofluid, explains itself, assuming nano as a system that is specified at the level of 10^{-9}m, and fluid as the form of matter that continually deforms itself under applied shear stress. The application of nanoparticles as a carrier medium in fluid produces nanofluid. This nanofluid consists of particles that exhibit Brownian motion when they are dispersed in the fluid. The use of nanoparticle enhances the properties of the fluid. These properties are physical[1, 2], rheological[3-6], electrical[7], chemical[8, 9] and biological[10-12].

There has been lots off nanofluids experimental studies. These studies are related to metal, metaloxides, ceramic and polymeric nanoaprticles dispersion in different base fluids. The nanofluid experimental studies have tried to undermine different properties of basefluid modification with nanoparticles. These properties are thermal conductivity enhancement, viscosity change, particle sizes, zeta potential, density, heat capacity, heat flux, electrostatic and Van der Waal forces, pH variation, and many others. Variable parameters are too many and increases with changing nanoparticles being used. The extent of extracting different parameters with experimentation requires high technical expertise, as well as, requires extensive material usage for accuracy of data prediction and extensive time period for performing each experiment.

Different experimental studies for nanofluids have been done for more than two decades. The Argonne Lab in United States under the supervision of Dr. Stephen US Choi was the first to call new heat transfer fluid as "Nanofluids"[13, 14]. Further, various researchers started to undermine distinctive properties of nanofluids in different conditions. The outbreak of usage was not just held in the engineering sciences; whereas, it became popular in biological science and pharmacology. The enhancement of the properties was immense as compared to the amount of particle concentration being used. The investigated study shows that Al_2O_3 nanoparticles when used at a volume fraction of 1-5%, shows 60% increment in the viscosity of water[15]. Then CuO nanoparticles have been investigated showing an increase of viscosity by 60-80% in water based nanofluid[16]. Later other nanoparticles were also examined for enhancing viscosity, thermal conductivity and other proeprties[17-21]. The usage of nanoparticles in biological basefluids enhances the properties of fluid. This nano-biofluid received a huge importance from the medical side for diffusing the Gold nanoparticles in different fluids to treat cancers[10].

However, as discussed that there have been immense experimental studies on the dispersion and application of nanofluids; nevertheless, conducting these experiments is being considered as an expensive and time consuming method. Further, predicted experimental results are genuine, on the contrary, they require lots of effort and knowledge on experimental procedures. Due to these drawbacks and upcoming computer age, researchers are more diverting the experimentation on simulation platforms. Therefore, since the last decade due to enhancements in molecular dynamics and computational technology, nanoparticle dispersions in different fluid's simulation are being attempted. By conducting the dispersion of nanoparticles in fluid using MD has become a useful and cost-effective approach. MD has become popular for nanofluids simulation on a large scale since the last decade as tabulated in table2. Before this, there were MD simulations, but they were mostly related to self-diffusion of fluids[22], mixing of oil with water to create emulsions, protein bi-layer [23]and polymeric diffusions [24].

The increase in the nanofluidic simulations is due to the concern and curiosity of how the diffusion of nanoparticles takes place in different fluids. These simulations can easily be used to understand the pheonomena and further analysis. The electrostatic, Van der Waal, electrosteric and Derjaguin and Landau, Verwey and Overbeek (DVLO) theory can further be understood by simulation, which were hard to understand at the

time of experimental studies. Moreover, the visualization of the simulations can explain the transport of the nanoparticle in fluid on the greater scale; this is a necessary fact to understand the diffusion of nanoparticles, since it differs from its microparticles counterparts. Thereby, lots of researchers came up with different techniques to design nanoparticles fluid interactions; some came up with their own potential and some used already available techniques. Nevertheless, these applied techniques and methods were progressive in describing the nanoparticle interaction with different fluids. Furthermore, researchers have also tried to use various simulation packages.

The initiative was mostly started with describing the system dispersion and diffusion with the Brownian equation of motion that is interconnected with Einstein diffusion model as shown in equation 1 and 2.

Later, Stokes formulation was also incorporated for enhancing the results. Moreover, the derivation for Newton's formulation indeed starts from the Langragian formulation that was further optimized by the Galilean relativity principle. This derivation is the bases for the molecular dynamic simulations to analyze the detailed atomic motion within the MD domain rather than just implementing the statical analysis [25]

$$F_i = m_i a_i \qquad (1)$$

$$m_i \frac{d^2 r_i}{d_i^2} = -\frac{dV}{dr_i} \qquad (2)$$

F_i force on particle i, m_i mass of particle i, a_i acceleration of particle i, r is the position vector and V is the potential energy derivative. Equations of motion are time reversible; if we change the signs of all velocities, the atoms will retrace their trajectories. Furthermore, numerical methods are required to solve these equations for systems larger than two independent particles.

However, this review demonstrates the simplicity for adopting the MD technique for nanofluid simulations. Further it describes to the reader, the easy procedure for carrying out these simulations. There are different reviews on MD, but they are mostly oriented towards biological or protein simulations. Further, this review has gathered previous studies carried out by others on various nanofluid simulations using different methodologies as shown in table 2.

II.   SIMULATION METHODOLOGY

The process followed by the molecular dynamic simulation technique equilibrate the system from its unstable position to stable position. Implementing force field causes the movement of the atoms in the system. Later, the pair potential, computes a particular behavior that is required to fulfil the simulation. The movement of particles in the system is caused by the velocity theorem, i.e. carried out by ensembles. These ensembles help to carry out thermodynamic conditions on a system using the kinetic theory of a molecular system; this theory further causes the system equilibration with time interval. Furthermore, the system is equilibrated for different

time intervals, i.e. the number of runs to equilibrate the system. Additionally, the minimizations are used to re-orient the particle configurations for energy conservation. After the successful equilibration runs, the data is analysed for convergence and experimental comparisons. Further the mechanism is illustrated in Figure1, i.e. a flowchart of MD simulation steps.
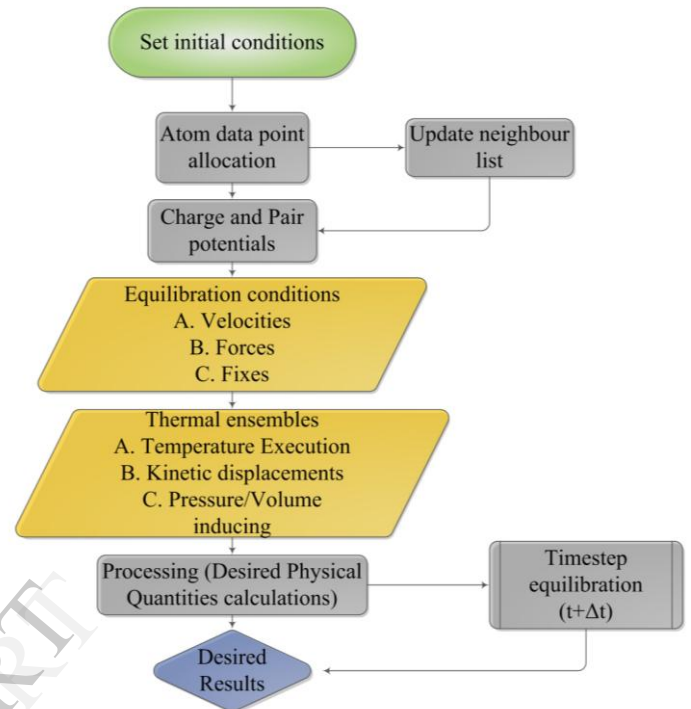

Figure 1 Flow chart of step-by-step procedure of molecular dynamic simulation.

III. ATOM SETTINGS/ PREIODIC CONDITIONS

The atom settings are the set of data that specifies the atom positions in the domain, where molecular interactions will be taking place. Atom settings, in particular, describe the x, y, z positions of one particular atom in three-dimensional spacing or lattice. Initially, if the system contains atoms that are going to be simulated for a nanofluid simulation, it is better to achieve their protein data bank files and use Packmol to pack both the files together in a specified lattice with a reasonable distance between the interacting atoms. Initial PDB can be generated by either Accelrys Material studio Ltd. or any convenient software that is capable of doing this; such as ChemDraw, Crystal maker, JMol and Avagodros. After setting atoms coordinates, the system is simulated in a periodic boundary condition.

An infinite lattice constructed to replicate the cubic simulation box throughout the domain referes to periodic boundary condition. Atom settings in a center box replicates and is a mirror image for the settings in other boxes as shown in Figure2. A disturbance in one box matches in the other box. Atom leaving from one box enters the other neighbouring box from opposite position. Subsequently, the central box is free of any boundaries.
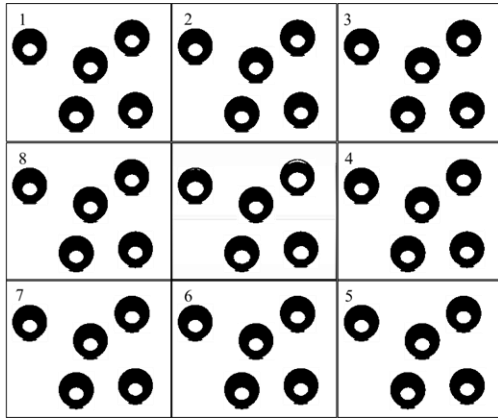
Figure 2 Periodic boundary replication.

IV. FORCE FIELDS

The force field is a basic step to describe the interactions between atoms and their potential energies. Furthermore, force fields can be constructed by parameters achieved from the potential energies using the apparatus such as experimental data of x-ray electronic diffraction, Nuclear magnetic resonance (NMR) and Fourier's transformation infrared (FTIR) spectroscopy; which gives the differentiation between matter and radiation with the uses of semi-experimental technique of quantum-mechanical calculation. Moreover, force fields are obtained parameters from higher-level quantum-mechanic calculations. These calculations help in imitating the realistic performance of the atomistic system with which results of interactions can be achieved in a matter of time. However, a successful simulation performance depends on the rationality of force fields being used.

Further, the computation of classical energy terms is carried out using force field. These terms account for the calculation of interaction parameters as shown in Equation 3. Later, this equation is elaborated for further understanding by graphical representation as shown in table1, with its specific variable descriptions.

$$U = \sum_{bonds} \frac{1}{2} k_r (r - r_0)^2 + \sum_{angles} \frac{1}{2} k_\theta (\theta - \theta_0)^2 + \sum_{torsions} \frac{V_n}{2} \big[1 + \cos[n_i(\varphi_i - \varphi_{0,i})] \big] +$$
$$+ \sum_{elec} \frac{q_i q_j}{r_{ij}} + \sum_{Pairs, ij} [\varepsilon_{ij} \left(\frac{r_{0,ij}}{r_{ij}} \right)^{12} - 2\varepsilon_{ij} \left(\frac{r_{0,ij}}{r_{ij}} \right)^6] \qquad (3)$$

The scientific calculation of parameters such as k-bond, k-angle, and k-torsion are known as potential energy functions[23]. The subject in simulation depends on its force field, on the other hand, the way which van der Waals and electrostatic interaction are treated, determines the precision of the computational simulation. Additionally, the force fields that have generally been used are 'Amber, CHARMM, OPLS and Gromos'.

However, for the interatomic collisions, force field implements interaction parameters of scientific measurements used to show the potential energy arrangement of elements. To sum up, force field actually holds parameters that are controlled from equally experimental observation and large amount of quantum-mechanics calculation.

The interacting bond expressions are well explained by the non-bonded van der waals and coulomb's forces between the atoms. The angles terminologies and torsion technique may be implemented to the corresponding angular coordinates from the stationary point of a classical diffusion equation. However, terminologies represent a different primary condition for diffusion. In addition, the variety of potentials states the degree of diffusion space in a system. On the other hand, another method to compute the diffusion coefficient for each terminology are outlined by interaction potential. Non-bonded force parameters of larger range interactions can be estimated from the comparative values of the experimental work for the Van der Waal and coulomb's parameters.

There are many force fields that give suitable parameters for mimicking the realistic effect of nanofluid, out of which some are aimed at each and individual atom in a system. However, other relate to the whole molecular arrangement. Furthermore, different types of force fields that has been used and are being used for nanofluid simulations are given in section 3.A.

A. Types of Force Fields

There are many force fields that are widely being used for nanofluids such as *amber, charmm, compass, opls, gromos, COMPASS, EAM* and *MEAM*.

A.1 Universal Forcefield(UFF):

Most particles have a force field that gives a parameter aimed at each and individual molecule in a system. If, integrating hydrogen with combined atoms of carbon, force fields that handles hydrogen and carbon atoms in each part of methyl are controlled by Universal force field. This is a force field distinctive from others, as it covers all the periodic table elements. The parameters are an estimation from general rule; that is used to convert the elemental parameters into intermolecular interaction parameteric values for calculation.

It is hard to obtain consistensy of results using UFF to that of experimental ones. Therefore, it is not convenient to use this force field for condensed state calculations. Nevertheless, this forcefield is good for exotic molecules for which other forcefield can not be implemented.

A.2 Amber:

Amber forcefield full abbreviation is Assisted Model Building Energy Refinement, which is a model created with energy refinement. Also a collective property of package that agrees us to convey out MD simulatons. Amber has a set of molecular mechanical force boundary conditions of bio-molecule. However, to use AMBER force field it is vital you have the dimensions for the parameters regarding the force field. Additionally, it is necessary to check on the charges of the atoms and force constant. Further, Fig.3 shows the use of AMBER forcefield to simulate stacked pyrenes that was carried out by S.M. Langenegger et al.
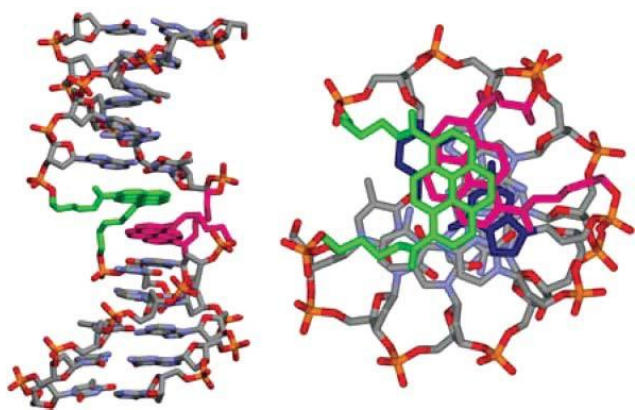
Figure 3 AMBER Molecular model of the duplex 3c*4c with two interstrand stacked pyrenes (HyperChem2 7.0, minimised with amber force field).15 The nonnucleosidic building blocks are highlighted in red and green. Left: view perpendicular to the helical axis. Right: view along the helical axis. Showing the pyrenes stacked on the nucleotide bases; nucleotides on the viewer's side have been omitted for clarity; the GC-base pair adjacent to the pyrenes is shown in blue [26].

A.3 Chemistry At Harvard Macromolecular Mechanics (CHARMM):

CHARMM that consumes several properties of charm force fields such as *CHARMM19, CHARMM22*, and *CHARMM27*. In molecular dynamic these are the most popular types of charm force field. This force field helps in protein simulations[27]. Later, it was also used for gold nanoaprticles simulation with peptides[28]. Furthermore, these are mostly used for protein system, but the drawback of this force field is it can calculate non-bonded parameters.

A.4 Condense Optimized Molecular Potentials for Atomistic Simulation (COMPASS):

Moreover, *COMPASS* is a unique technique which is considered as a force field that provides atomistic simulation for reduced materials. Compass means condense optimized molecular potentials for atomistic simulation[29, 30]. These force fields permit perfect concurrent estimation of structural, conformational, vibrational and a thermo physical property which may occur for a vast range of molecular separation in condensed phases, and with a confined range of environments[31]. Later, Fig.4 a,b shows the use of COMPASS force field for phenol and carboxylic andhydride simulations [32] and Fig.4c demonstrates the use of this forcefield in simulating metaloxide nanoparticles in aqueous fluid[33]. Further the use of COMPASS forcefield for molecular dynamics of polymer metaloxide system was also proposed by Prathab et al. [34] .
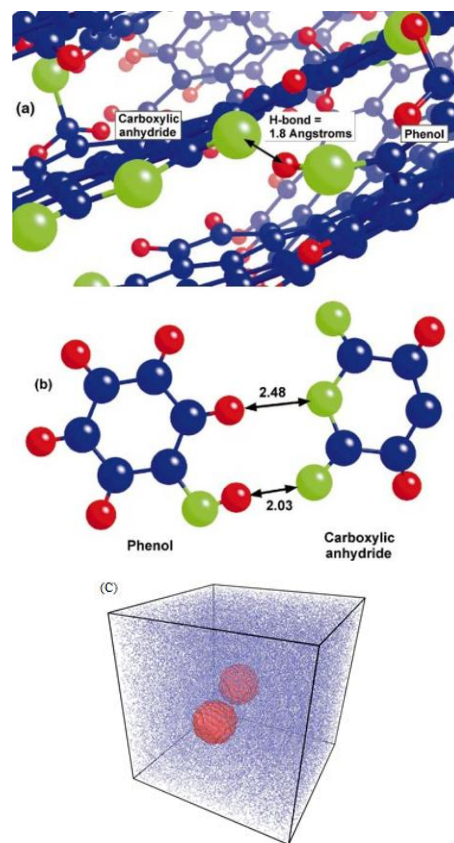

Figure 4 (a)A close-up view of H-bonding between a phenol group and a carboxylic anhydride group as predicted from the MD simulations of soot with the COMPASS forcefield; b) MP2/ 6-31G* calculation of H-bonding between phenol and carboxylic anhydride used to test the result of the COMPASS-based MD simulation shows similar H-bonding behavior [32];c) CuO (metaloxide) nanoparticles simulated using COMPASS forcefield[33].

A.5 Optimized Potentials for Liquid Simulations (OPLS):

OPLS is a force field which is divided into two different sections one being united atom which stands for *OPLS-UA* and the other being *OPLS-AA* force fields. However, the basic definition of OPLS is optimized potential for liquid simulations. *OPLS-AA* force field is used for renovating the Fourier torsional coefficient. This renovates the accurate data as an aim proficient fitting subspace of the entire potential energy surface. Thus, setting weights for each of the fitting focuses dependent upon sizes of the potential-energy slope. *OPLS-UA* [35] is use for possible flattening in standard *OPLS-UA* constraint with modification to Van der Waal forces and improper torsion terms.

A.6 Gromos

Gromos is a general force field that holds information of biological molecules in a process[36]. Furthermore, it integrates its specific force field maintaining protein, nucleotides and so forth. It can be utilised to chemical and physical nature ranging from glasses and liquid crystal to polymer and solution of biological particles. This force field is highly fast due to algorithms as it runs accumulates times faster than other force feilds.

The Gromos force field vary between the rests in the way hydrogen atoms are preserved. Furthermore, in the gromos

force field's non-polar hydrogen atoms are reviewed into their adjacent carbon molecule, i.e. a three particle H-C-H combination, which formally becomes a single CH2 molecule. Moreover, this form of force field is called a combined atom and is more effective for simulation of lipid membrane.

A.7 Embedded Atom Model/Modified (*EAM/MEAM*)

EAM is a force field that describes and estimates the energy between two atoms. In this case energy can be known as a sum of a function of departing between two atoms and its neighbours in the system. Furthermore, EAM is mostly associated for a metallic process and is very commonly used in molecular dynamics simulation[37].

Moreover, the modification of EAM has already been carried out as MEAM, which stands for modified embedded atom method. This forcefield is a semi practical derivation method developed to calculate the properties of a metallic process. Additionally, this technique has demonstrated to be accurate in terms of prediction bulk and surface properties within metals. Modern modification of this forcefield has helped to use large atoms and elements in the system.

V.   PAIR POTENTIAL

Pair potential is a process where a function portrays potential energy of two particles in interaction. Furthermore, Pair potentials interlinks with one law which is recognised by lennard-Jones potentials law denoted by equation (4).

A.   Lenard Jones(LJ) Pair potential

LJ potential is an estimation which portrays the potential of interaction among two non-bonding particles in respect to the distance of distribution of atoms. Atoms that consist of same mass and molecular diameter interact by Lennard-Jones potentials.

$$J = 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - c_{ij} \left(\frac{\sigma}{r_{ij}} \right)^{6} \right] ; \ i,j=[1,2,3,...] \quad (4)$$

Where J is intermolecular potential between two atoms. ε is how strong the particles are attached. σ is how close they can approach each other. r is the distance of distribution of particles. Consequently, LJ potential has many drawbacks that can either put the simulation in danger or enable to give you the perfect results. Such as, it only has two parameters, therefore can only be accumulated into only two physical quantities. Eventually, this can be an issue to satisfy three different interacting atoms in the system. As the scaling of energy and bond elasticity after considering this ideology is difficult to pair all three quantities together with L-j potential.

B.   Brownian potential

Brownian potential is the random motion of molecules projected in a liquid [38] leading to their collision with fast atom in solid and liquid state. This potential can be devoted to mathematical model in simulation to configure the random movement. Brownian potential also describes the diffusive limit of the Langevin equation where the motion is highly random. However, this potential has a high friction coefficient. Brownian helps in expressing processes as diffusion controlled system.

C.   Smoothed Particle Hydrodynamic (SPH) potential

SPH is an abbreviation for Smoothed Particle Hydrodynamic which is a computational technique used for the simulation of fluid hydrodynamics[39, 40]. Furthermore, it applies mesh free method, where motion is not restricted. In simulation of fluid dynamics this is highly used, as SPH assures conservation of mass without further computation since the molecules state the mass itself. Moreover, it has a feature which computes pressure from weighted pressure distribution of neighbouring function rather than solving linear parts of the system. Furthermore, this potential promotes hydrodynamic effect in the system. Thus, fulfilling the hydrodynamic movement of molecules according to the liquid-liquid layering[41].

D.   Dissipative particle dynamic (DPD) potential

DPD is used to perform stochastic simulations [42, 43]. This potential helps in simulating Brownian dynamics of complex fluid system. This method was used to neglect lattice properties for the lattice gas automata and attempt hydrodynamic time and space with in molecular dynamic boundaries. Furthermore, DPD involves a set of molecules moving in the continuous scale of the time and space. Momentum of conservation of energy necessitates that random forces applied when two beads are not symmetrical. Moreover, pairs of molecules interacting take the help of a single random force calculation. This differentiates DPD to Brownian dynamics in how each individual particles experiences random force independently of all molecules.
Additionally, two particles get so close they can be considered to be known as zero potential energy. Moreover, the space of distribution decreases as the chances of interaction increased and in some way the potential is decreased from zero to negative as the particles held together. However the length among the base will remain constant to reduce the atoms to gain a balance which can be estimated by the separation distance, these values are used for acquiring coefficient of pair potentials.

VI.   ENSEMBLES

Molecular dynamics simulation is attempted under pre-defined thermodynamic conditions, such as constant number of particles (N), volume (V), pressure (P) and temperature. These conditions specify the "ensemble" of the systems. Ensembles are a compilation of every possible classification which contains different microscopic properties that include a

similar macroscopic or thermodynamic quantities. Mostly, a mathematical quantity used to combine sums of motion in Molecular dynamics is fulfilled using algorithms (used in computing). Therefore if every force in the boundary found from Newton's formula of activity, this will be connected to the impending source of energy of the boundary then the total energy of the process is given by equation 5.

$$E \;=\; K_E + P_E \qquad\qquad (5)$$

A. Types of Ensembles

There are three major types of ensembles a) Micro canonical ensembles NVE; b) Canonical ensembles NVT and c) Isothermal-isobaric NPT

A.1 Microcanonical Ensembles

Microcanonial ensembles, is a natural ensemble. This is the first ensemble used for describing conservation of energy in a system. Microcanonical ensemble further is a forms of an algebraic ensembles which can be applied to represent the potential conditions of a mechanical group which has total energy. Therefore, the system is known to have been isolated in the intelligence that, process cannot change or exchange energy or particles with its boundary, as the energy in the process stay constant known to time. The development of energy composition is kept in the same natural property. The variables of the NVE ensembles are numerical values of particles (N), the volume (v) and the last letter is (E) which stands for total energy.

A.2 Canonical Ensembles

Canonical ensembles are a form of statistical ensemble that can be used to show the natures of a mechanical property which is thermally equal with the high temperature bath. The process of the mechanism is said to be clogged in the sense that the boundary can change energy from opposite directions. Therefore, various chances to remain in normal states of total energy. The process composition or shapes are kept the same in all possible forms according to the process. The adjustable variables of the canonical ensembles are the absolute temperature known as T. This is dependent on mechanical variables such as N which stand for the quantity of particles and lastly V being volume, i.e. base x height x length therefore, summing NVT ensembles. This ensemble make the system volume constant varying the system pressure.

A.3 Isothermal-isobaric Ensembles

Isothermal-isobaric ensemble has constant temperature and steady pressure ensemble is a statistical mechanics ensemble that remains the same in terms of temperature and P which is known for pressure gives NPT ensemble. This ensemble is highly used in chemistry, for its effects are normally taken out under constant pressure conditions. Ensembles have been used for many things and have been measured through two simple schemes; one being algorithm and another being Monte Carlo simulation. It was an old process used for bio molecules. On the other hand multibaric-multithermal algorithm has two

dimensional casual chances not only in a potential energy space but also in the system required. Therefore, the algorithm has a higher potential sampling efficiency than the multicononical and canonical algorithm.

VII. PROPERTIES RELATED TO NANOFLUID DISPERSION

Properties analysed for dispersion analysis of nanofluid suspension are mostly related with four important parameters a) diffusion coefficient, b) Radial distribution function (RDF) c) viscosity and d) thermalconductivity. Out of these four properties diffusion coefficient, RDF and viscosity defines the system agglomeration and dispersion status of particles in fluid suspension. Diffusion coefficient is related to the molar flux due to atomic diffusion, further, it is defined by a slope of concentration of the sample.

Viscosity is the property that defines deformation of the material due to applied shear stress. RDF is the pair distribution function, that adheres to the system density variation with respect to the molecular spacing. RDF also defines the crystallinity structure. Finally, thermal conductivity is a property that defines the heat conduction, moreover, correlated with fourier law of conduction. The equations used for these four parameters for molecular dynamics calculation are given in table 3.

VIII. RECOMMENDATIONS AND SUGGESTIONS

The implementation, importance of molecular dynamics can now be a valid point for researcher to simulate nanofluids; rather than experimentally testing the properties of nanofluids. Nevertheless, experimentation cannot be completely neglected, but simulation sometime requires initial proper validation of parameters with realistic experimentation. The recommendations to the reader is to consider the following steps or softwares to simulate the on purpose nanofluid simulations. Fig. 5 demonstrates different softwares and their capabilities as a part of nanofluid simulation criteria.

1) The nanofluid atom coordination files can be generated by a software that can easily make a PDB file.

2) Later the nanoparticle can either be made over the Material studio software or Visual molecular dynamics (VMD).

3) Further, after creating the nanoparticle PDB file, it can be used in Packmol software with the solvent file to combine them together. This takes quite a while, however, it arranges the nanoparticles within the dimensions specified to the Packmol.

4) Now, as we have obtained the complete PDB (i.e. Solvent + nanoparticles) we need to assign a forcefield and intermolecular potentials that can either be carried out using VMD or Material studio by discover tool.

5) After this, the complete atom settings data output file is exported in a correct format according to the source code simulation software that can read it.

6) The simulation script is written on a particular source code for simulating the system.

7) Later, this script is executed on the source code software, where further trajectories and output results are computed.

8) For visualization of the simulation output trajectories can be carried out using one of the visualization software mentioned in the figure 5.
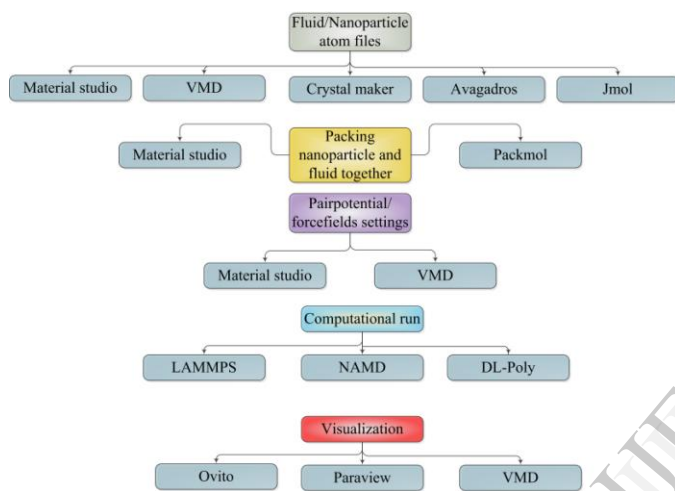

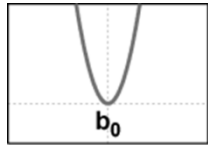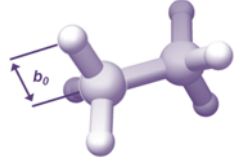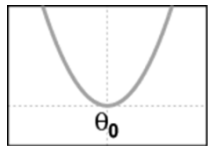Figure 5 Softwares for attempting nanofluid simulations.
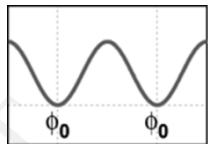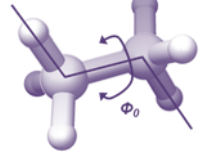
IX. CONCLUSION

Simulations have become a hard-core element for modern world sciences. Science that lay behind experimental aspects to be performed over a computer are known as simulations. These way simulation that are used to simulate the virtual reality dynamics at an atomic or molecular level are "Molecular dynamic simulations (MDS)". MDS/s are being used for last 50 years. This has gained pace over the time and now due to its flexibility and cost effective nature, it is being implemented in biological and life scien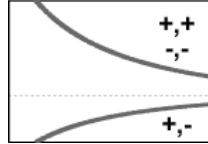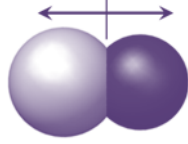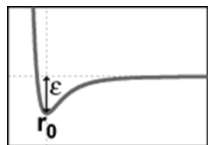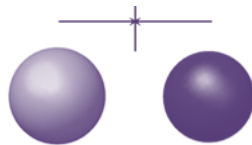ces, engineering and material sciences, and nanotechnology. MDS has helped researchers to excavate further understanding of different phenomena's at atomic level such as rheology, tribology, stress and strain analysis of fatigue material, Brownian motion and thermo-physical quantities. It has become a breakthrough in understanding the different phenomena's that were not easy to understand while performing the actual experiment. The quantitative analysis done by the help of various algorithms excavates underlying features that were hard to define before. The rheological, thermo-physical, tribological and material science properties are further being polished by MDS since it has become easy to undermine the different aspects of experimentation.

However, this study has brought the way of conducting nanofluid suspension MD simulations using different softwares, and the way it can be visualized. Therefore, nanofluid simulations are gaining wide recognition due to verstalitiy and cost-effectiveness.

The computer age is making people dependent on the simulations, this review can be a great help for researchers interested in simulating nanoparticle dispersion in various engineering or biological fluids.

Table 1. Force field classical energy function.

Equations	Energy calculation methods	Graphical illustration	Variable resemblance
$\sum_{bonds} \frac{1}{2} k_r (r - r_0)^2$	Bond stretches	b_0	
$\sum_{angles} \frac{1}{2} k_\theta (\theta - \theta_0)^2$	Angle bending	θ_0	
$\sum_{torsions} \frac{V_n}{2} \left[1 + \cos[n_i(\varphi_i - \varphi_{0,i})] \right]$	Torsional rotation	ϕ_0 ϕ_0	
$\sum_{elec} \frac{q_i q_j}{r_{ij}}$	Electrostatic interaction	+,+ / -,- / +,-	
$\sum_{Pairs,ij} \left[\varepsilon_{ij} \left(\frac{r_{0,ij}}{r_{ij}} \right)^{12} - 2\varepsilon_{ij} \left(\frac{r_{0,ij}}{r_{ij}} \right)^6 \right]$	Van der Waal-interaction	ε r_0	

$$\alpha + \beta = \chi. \qquad (1)$$

Table 2. Nanofluid simulations historical background and applications for different systems.

S No.	Simulation	On What	Forcefield/ potentials used	Year	Properties Analysed
1	Adil Loya et al. [33]	CuO in water	COMPASS forcefield, DPD potential and SPH potential	2014	Viscosity and diffusion properties
2	Ali Rajab pour et al. [44]	Cu water simulation	L-J potential and Lorentz-Berthlot	2013	Specific heat capacity
3	Hongbo et al. [45]	Cu-Ar Ar-Ar	L-J Potential	2012	Diffusion
4	Ali Mohebbi [46]	Beta-Si3N4 in argon system	L-J Potential, Morse function and Charm FF	2012	Thermal conductivity and specific heat
5	Yung Sheng Lin et	EthyleneGlycol-Cu	L-J Potential,	2012	Thermal

	al. [1]		Morse potential, Lorrentz Berthelot mixing rule and JR FF		conductivity
6	Wenzheng Cui [47]	Cu in argon liquid	L-J Potential	2011	Turbulance model
7	Valery Ya Rudyak et al. [48]	General Np in dense fluid	L-Jpotential and R-K Potential	2011	Coupling factor
8	Chengzhen Sun et al. [37]	Cu-Ar nanofluid	L-J Potential and EAM potential	2011	Thermal conductivity
9	D.L Cheung [49]	Nanopartilce-solvent	L-J potential	2010	Diffusion and RDF
10	N.Sankar et al. [50]	Pt-water and pt-pt	L-J potential, Morse potential and FENE potential	2008	Thermal conductivity
11	Wen-Qiang Lu et al. [51]	Alumina-water or C2H5OH or C2H4(OH)2	L-J potential	2008	Thermal conductivity and viscosity
12	Ling Li et al. [52]	Cu-Ar	L-J potential	2008	Thermal conductivity
13	S. Sarkar et al. [53]	Cu-Ar	EAM and L-J Potential	2007	Thermal conductivity and Diffusion
14	Mingxiang Luo et al. [54]	Hydrocarbon-water-polymer Np	Gromos force field and L-J potential	2006	Density and diffusion
15	Delphine Barbier et al. [55]	PEO Oilogomers melts with silica nanoparticles	L-J potential, UFF and OPLS FF	2004	Density and RDF
16	Francis W. Starr et al. [56]	Polymer melt with np	L-J potential and FENE model	2002	Density and RDF
17	Anatoly Malevanets et al. [57]	Nanocolloidal model	L-J potential	2000	Velocity Autocorrelation Function (VACF), Diffusion
18	D M Heyes et al. [58]	Colloidal model	WCA and L-J potential	1998	RDF, VACF, Density and diffusion

Table 3. Nanofluid simulation dispersion properties equations used in most molecular dynamics calculations.

Property	Definition	Statisical Mechanical formula	Einstein Relation for larger t
Diffusion Coefficient	$\dot{n} = -D\dfrac{\partial n}{\partial x}$	$\dfrac{1}{3}\displaystyle\int_0^\infty \langle v_i(t).v_i(0)\rangle dt$	$\dfrac{1}{6t}\langle |r_i(t)-r_i(0)|^2\rangle$
Thermal conductivity	$q = -\lambda\dfrac{\partial T}{\partial x}$	$\dfrac{V}{K_B T^2}\displaystyle\int_0^\infty \langle \tilde{q}_\alpha(t).\tilde{q}_\alpha(0)\rangle dt$	$\dfrac{V}{K_B T^2 2t}\langle (\delta\varepsilon_\alpha(t)-\delta\varepsilon_\alpha(0))^2\rangle$
Shear Viscosity	$F = \mu\dfrac{\partial U}{\partial x}$	$\dfrac{V}{K_B T}\displaystyle\int_0^\infty \langle \tilde{p}_{\alpha\beta}(t).\tilde{p}_{\alpha\beta}(0)\rangle dt$	$\dfrac{V}{K_B T 2t}\langle (\tilde{D}_{\alpha\beta}(t)-\tilde{D}_{\alpha\beta}(0))^2\rangle$
RDF	$g(r) = \dfrac{dn(r)}{\rho 4\pi r^2 dr}$	$g(r) = \exp\left[-\dfrac{u(r)}{K_B T}\right]$	None

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Abbreviation Table and their units

Symbols	Meanings
CuO	Copper Oxide
CuO-NP/s	Copper OxideNanoparticle/s
DLVO	Derjaguin and Landau, Verwey and Overbeek
EAM/MEAM	Embedded Atom Method/Modified Embedded Atom Method
LJ	Lenord Jones
NVE	Number of atoms, Volume and Energy
NVT	Number of atoms, Volume and Temperature
NPT	Number of atoms, Pressure and Temperature
UFF	Universal Forcefield
AMBER	Assisted Model Building Energy Refinement
CHARMM	Chemistry At Harvard Macromolecular Mechanics
COMPASS	Condensed-phase Optimized Molecular Potential for Atomistic Simulation studies
OPLS	Optimized Potentials for Liquid Simulations
DPD	Discrete particle dynamics
MD	Molecular dynamics
BD	Brownian Dynamics

SPH	Smoothed Particle hydrodynamics
r_{ij}	i-j atomic separation distance.
$\hat{r}_{ij}$	Force in particular directions
d_t	Timestep size
K_B	Boltzmann constant
T	Temperature
t	Timeperiod
F	Magnitude of Force
$\dfrac{\partial U}{\partial x}$	Velocity in x-direction
$\dot{n}$	Diffusion flux
D	Diffusion Coefficient
$\dfrac{\partial \phi}{\partial x}$	Molar concentration in x-direction
$r_i(t)$	radius of particle i at time t
$r_i(0)$	radius of particle i at starting time
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
μ	Viscosity
TEM	Transmission Electron Microscope
J	intermolecular potential between two atoms.
i	Particle i
j	Particle j
ε	Strength of particle/ Dielectric constant
σ	Distance between interaction
r	Distance of distribution of particles.
q	Charge of particle
θ	Bond angle
φ	Dihedral torsion angle
x	Out of plane angle
α	Gaussian number
ρ	Density
RDF [g(r)]	Radial distribution function