Chapter 5

Problems Faced While Simulating Nanofluids

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Additional information is available at the end of the chapter

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Abstract

Problems are faced when something is already been adopted for a considerable amount of time–here the problem that is discussed is related with nanofluids. The nanofluids have been considered for different engineering applications since last three decades; however, the work on its simulation has been started since last two decades. With the time, nanofluid simulations are increasing as compared to experimental testing. Researchers conducting nanofluid simulations do find difficulties and problems while trying to simulate this system. In addition to this, most of the time researchers are unaware of some basic problems and they find themselves stuck in relentless difficulties. Most of the time, these problems are very basic and can waste a lot of useful time of a research. Therefore, this chapter introduces some fundamental problems which a researcher can find while simulating nanofluids and with a simple way of dealing with it. Moreover, the chapter withholds lots of information regarding the way to design and to model a nanofluid system. Not only this, it also tends to elaborate the nanofluid simulation methodology in a precise manner. Moreover, the literature shows that nanofluid simulation has gained high consideration since last two decades, as experimental techniques are out of reach for everyone. In addition to experimental techniques, they are expensive, time-consuming and require high skills. However, it seems the simulation is picking pace with the due time and is considerably being adopted by the expertise dealing with nanofluids. This opens a high prospect of simulating nanofluids in future. Nevertheless, it seems there will be user-friendly software to conduct nanofluid simulations. Finally, issues and their resolution have also been conveyed which is the main aspect of this topic.

Keywords: nanoparticles, nanofluids, molecular dynamics, simulations, problems

1. Introduction

Couple of decades back, nanofluid research was mostly conducted using experimental techniques. With time, as the computational power acquired drastic developments, new algorithms were designed, and therefore, today, we have got sophisticated software and mathematical models to solve and simulate the nanofluid environment.

1.1. Background knowledge

Nanofluids comprises of two constitutes, i.e. Nano comes from nanoparticles and fluid comes from base fluid. The need of combining nanoparticles with fluid was necessary for enhancing the properties of the base fluid. Addition of nanoparticles to the base fluid helps in altering and optimizing properties such as physiochemical [1], thermo-physical [2], rheological [2–4], etc.; to give a new composite performance. The initial mixing of nanofluids can be dated back to the time of the US choi in 1995, he was the first one to form nanofluid at Argonne laboratories USA [5, 6]. He used the nanofluid for optimization of thermal conductivity. Since then there have been several experimental studies over the thermal conductivity analysis of different nanoparticles in various base fluids [5, 7–9].

By looking at thermal conductivity improvement, other researchers came up with different ideas and formulations for utilization of this technique in various fields of science. Today, nanofluids are being used in biological, pharmaceuticals and medicine [10], engineering [7], lubrication industries [11, 12]. The major work on experimental side in all these industries has been carried out; however, these experiments of nanofluid require high skilled labour and expensive equipment. Furthermore, material purchase and characterization are costly. Due to this, researchers and industrialists working with nanofluids are trying to develop a model that can replicate mechanisms dealing with nanoparticle and fluid interactions. However, this subject is wide and requires huge expertise to deal with.

Currently, as the computational power has enhanced to a level where people are finding it easy to simulate and replicate systems within their personal computers, it is now becoming quite manageable task to simulate nanofluids. But the task is not as simple as it seems, it requires a lot of understanding of physiochemical interactions with thermo-physical boundary conditions. There are many algorithms and mathematical models to be considered. As the number of these models and algorithms increases, higher the computational power is required for solving. Nevertheless, the endless applications and usage makes it convincible for an end-user to adopt this creativity, as it enables one to understand the process and makes it visually quantifiable.

Before moving forward, it is necessary to understand some basic theory that is behind the dispersion of nanoparticles within a certain fluid.

1.1.1. Theory behind dispersion of nanoparticle

Dispersion of nanoparticles is a process in which they are dispersed in a medium like fluid. These fluids are of different grades such as biological, aerospace, automotive and buffering solutions. According to the kinetic theory of molecules, as the molecule interacts with other molecule, it starts to generate some heat due to kinetic molecular movement of the particle. This movement is accountable for the dispersion of nanoparticles in different fluids; thereby, this model causes anomalous increase in the heat transfer of the nanofluids. Furthermore, using this model, four major effects produced by nanoparticles dispersion can be explained i.e. (a) Brownian motion of nanoparticle, (b) liquid layering at liquid particle interface, (c) nature of heat transport between nanoparticles and (d) the clustering effect of

nanoparticles in fluid. These factors are responsible for inducing random motion within particle and liquid layers, and this phenomenon is Brownian motion. During the interaction between nanoparticle and fluid, heat is evolved, causing nanoparticles to cluster and agglomerate. These mechanisms have already been replicated by various researchers for analysing properties such as; (a) rheological, (b) thermo-physical and (c) physiochemical as mentioned in Section 1.2.

1.2. Applications

There are various applications in the area of nanofluid simulation. Currently, nanofluid simulation is being applied for analysing the rheological properties of nanofluid environment, which is useful for biological, oil and gas, lubrication and chemical industries. Now, by the help of simulation, it is possible to test those undesirable conditions that could not be tested before, such as testing viscosity at low and very high temperatures. Properties of ideal nanofluid can be tested and their results can also be validated using autocorrelation functions for satisfaction.

The use of molecular dynamics has enabled us to test and quantify thermo-physical quantities of nanofluid at obnoxious level. The chemical interactions that were complicated to understand from the real interface, now it has become straightforward to know how the atoms of fluid and nanoparticle interacts together, nevertheless, Brownian dynamics is more appreciably demonstrated and visualized. Having this all, analysing different properties of fluid and nanoparticle interaction, now it is easy to know other parameters such as specific heat [13], total energy, bond formation at molecular level, chemical interactions, etc. [14]. Furthermore, various effects that could not be judged by experimental testing can now easily be known such as the effect of liquid layering on thermal conductivity as investigated by Li et al. [15]. Particle effect on thermal conductivity analysis can now be determined as carried out by Lu and Fan [16]. Nevertheless, effect of surfactant addition in nanofluid system can also be tested using molecular dynamics, which can better tell about the chemical interaction and aggregation dynamics within this system as conveyed by Mingxiang and Lenore [17]. Rudyak also succeeded in showing that by changing nanoparticle size and shape effects the viscosity [18]. Therefore, by looking at the vast applications of nanofluid simulation, it is necessary to know some overview about how these simulations can easily be conducted.

2. The literature review

2.1. Need of simulations over experiments

Simulations are being preferred over experimental practices in the twenty-first century. As experiments require a lot of man power and material, which is costly and time-consuming, therefore, researchers are favouring simulations, as it saves material, money and time. With the advancement in computational technology, simulations are being approached to replicate the nanofluids. Simulations are not an old technique, and it has got a firm ground. Currently, the area of simulation to replicate the real phenomena of dispersion is through the

intermediate stages. Before moving to simulations, it is important to understand dispersion and interaction mechanism of nanoparticles with fluids. For this, the major phenomena that is used for dispersion is Brownian motion, which is an important aspect that controls the random factor of nanoparticle dispersion.

2.2. Simulations of nanofluids

Nowadays, the necessity of using simulation techniques is increasing due to its cost-effectiveness and time-saving capabilities. Simulations for nanofluids are mostly referred to as molecular dynamics simulation (MDS). However, before MDS, researchers adopted theoretical and numerical calculation method for computing thermo-physical quantities. Earlier theoretical formation, related to MDS research, has not established a strong hold position for replicating the mechanism of heat transfer, rheology and thermo-physics involved for nanofluid dispersion. This is because several researchers had modelled system using various assumptions rather using a definite formulation. This creates ambiguity in collecting results; however, they were well utilized for initial prediction of thermal transfer properties of nanofluid at the cost of wide inaccuracies. Experimental results that are representing actual system sometime are way off from the ideal method, in addition to this, researchers apply various differential equations for equating the system to realistic results as possible.

These methods are single-phase and two-phase methods [19] of nanofluid heat convection. They are still being used for predicting several properties related to heat transfer, convection and conduction within nanofluid systems [19–21]. Now these two methods are being embedded in computation fluid dynamic and molecular dynamics for heat transfer analysis [21]. The single-phase method of heat convection in nanofluid is an old method and is good for initial prediction of the thermal properties of nanofluid; however, the second-phase method is costlier as it requires higher computing power. In addition to the second-phase method, it is quite versatile as its prediction is in higher accuracy to the experimental results. Numerical approach simulates the nanofluid system using classical thermodynamics principles, which is more close to the single-phase model. Different correlations are applied to estimate the imbalance between the heat propagation values from actual to the ideal system. Physical interaction kinetics involved in real nanofluid system are not mimicked. This is why the real prediction is hard to achieve by this approach; moreover, two-phase fluid heat transfer involves higher mathematical complexity, which requires high computational power for general analysis of nanofluid heat transfer, rheology and thermo-physical quantities.

It was investigated by Sergis Antonis that due to not standardizing the procedure of nanofluid preparation diversifies accuracy of the experimental results obtained [2]. In this respect, MDS comes in to play, as it helps in simulating both nanoparticle and fluid particle system in one single domain, enabling us to mimic reaction kinetics of both materials in one single domain. However, these simulations require high computational power for simulating the system as it involves kinetic molecular movement of different atoms. Initially, MDS involved heat transfer within a nanofluid system in which it did not involve analysis with respect to the geometrical features or spherical with no surface texture. It used to be simple analysis in

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a uniform and homogeneous system. Earlier, properties of SiO_2 nanoparticles were calculated using Stillinger-Weber [22] and later fluid particles were represented by L-J potential.

There are two different dispersion prospects of MDS i.e. (1) non-equilibrium MDS (NEMD) and (2) equilibrium MDS (EMD). The macroscopic MDS mimics the molecular interactions between different molecules of various elements; in compound or ionic form. These different thermo-physical types of interactions of molecular dynamic quantities can be tailored and analysed by true boundary conditions. These boundary conditions are related to the physical settings, chemical interactions, charges, viscosity of the system and motion exhibition of particles. The interaction between the molecules is exhibited by Brownian motion as this mimics the random forces in the system. The system relies on different algorithms behind the scene to design a virtual nanoparticles dispersion in fluid. Furthermore, this is because the interaction kinetics of nanofluid system adhere with nanoparticle surface interacting with the surrounding fluid; this involves exchange of energy, surface tension between two, orientation of nanoparticle, surface energy, bonding configuration, nanoparticle dynamics and kinematics (including nanoparticle spin), liquid layering between nanoparticle and fluid molecule, and diffusion rate.

To explain the trajectories and velocities of a fluidic system, it is necessary to adopt a hydrodynamic framework. Computer simulations for mimicking trajectory of hydrodynamic dispersion of a dispersed particle in a fluid system was used by Ermak [23]. Nevertheless, Ermak and McCammon [24] work was more focused on the hyrdrodynamically concentrated system. The hydrodynamical system exhibited that the inter-particle distance is much greater than the range of hydrodynamic interactions. However, by implementation of Brownian dynamics by Ermak gave highly concurrent results with the experimental values achieved. The hydrodynamics of the system display combinations of Coulomb interactions; i.e. long range interactions as well as the Vander Waal interactions; short range interactions. Furthermore, the dynamics of the system is more convincing after applying the Derjaguin, Landau, Verwey and Overbeek (DLVO) [25] theory/factor in the system to mimic the charges and to enhance the realistic intermolecular attractions and repulsions.

Currently, there are different nanoparticles being considered for various applications. Therefore, for simulating nanofluids, modelling the nanoparticle is important, for that nanoparticle structure, shape and its properties should be known.

Subsequently, the mimicking of interaction potentials; i.e. using force fields such as embedded atom method (EAM), COMPASS, universal, etc; and the other forces between the atoms and molecules, the velocity verlet theorem is implemented. The velocity verlet theorem is a time-dependent movement of the atoms from one position to another using an algorithm for defining the movement, which is based on Brownian dynamics (BD). In addition to this, velocities or movements of atoms are controlled using thermal ensembles i.e. canonical (NVT), grand canonical (ΔPT), isobaric and isothermal (NPT) and micro canonical (NVE). These ensembles support in conducting thermal and physical perturbation to change the dynamical position of the atoms and molecules within a desired system. This causes the system to move to an un-equilibrium state. After starting and moving from an un-equilibrium state, the system is then equilibrated for convergence to equilibrium state. Finally, by this convergence,

the system acquires stability of temperature and physical quantity fluctuations. However, this convergence is an iterative process for which time steps are varied to achieve the real convergence results [26, 27].

Currently, there are various simulation of nanofluids, for example; CuO, TiO_2 and CeO_2 nanoparticle dispersion in water [3, 4]; furthermore, there are also studies of dispersing nanoparticles in hydrocarbons [28]. By having two different simulation strategies, a perspectives and robust methodology can be formulated. As these simulations are performed on two different types of fluids i.e. polar and non-polar, so a concurrent methodology for both fluids can be deduced. Furthermore, up to the date, investigators have carried out various researches on nanofluid MDS, in addition to this, last two decades of work has been cumulated in **Figure 1**. Following are the details of their work in the field of nanofluid simulations.

In 1998, Malevanets and Kapral [29] formulated a method for computing complex fluidic systems using H theorem, which helped in solving hydrodynamics equations and transport coefficients. Colloidal model and random stochastic movement algorithm was established using Brownian dynamics which was formulated by Lodge and Heyes [30].

Francis W. Starr investigated effect of glass transition temperature on the bead spring polymer melts with a nanoscopic particle. He found that the surface interaction dominates due to nanoparticle diffusion within the melted polymeric system [31].

Simulation of chemical interactions was also carried out, and the bond length and structural orientation was noted for Silica nanoparticles in poly ethylene oxide (PEO) oligomer system. By this study, Barbier et al. concluded that the silica nanoparticles influence structural properties of PEO up to two to three layers [32].

Mingxiang and Lenore worked on hydrocarbon surfactant in an aqueous environment with a nanoparticle diffused within this system. It was observed from interactions that the agglomeration created between water molecules and surfactant was independent of nanoparticle i.e. it does not matter whether it is present or not [17].

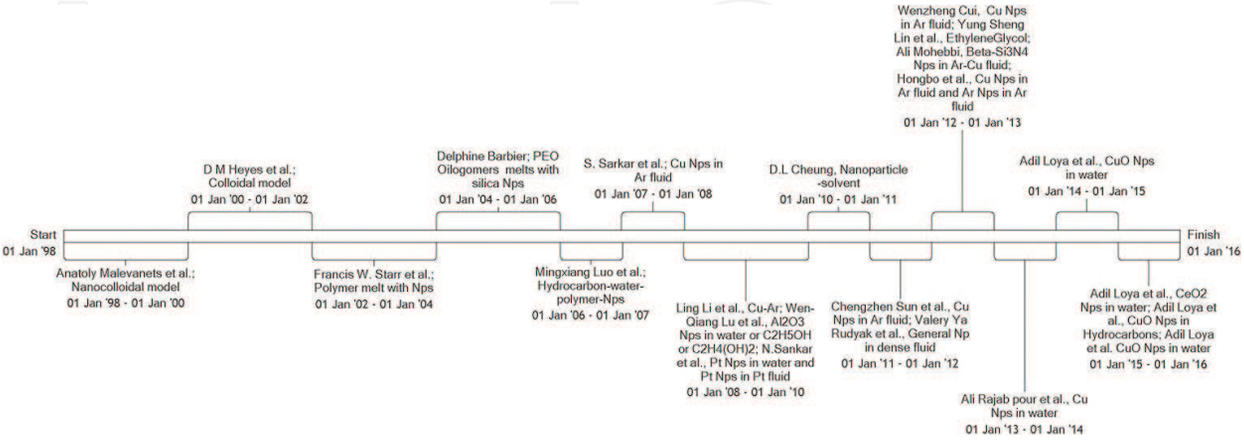

Figure 1. Timeline showing work carried out by different researchers since last two decades.

Sarkar and Selvam designed a nanofluid system of Cu nanoparticle and Argon as basefluid, for this, he used EAM potential and Green Kubo technique to find the thermal conductivity of this system. He examined that the periodic oscillation existed due to the heat fluxes imposed by Leonard Jones (L-J) potential [9].

Li et al. later worked on similar system of Cu nanoparticle with Ar base fluid; however, they investigated Brownian dynamics induces a thin layer around a particle, giving a hydrodynamic effect to the particle dispersion [33].

Lu and Fan investigated thermo-physical quantities of Alumina nanoparticles dispersed in water and concluded that the particle volume fraction and size effects the viscosity and thermal conductivity [16].

Sankar et al. examined and formulated an algorithm for calculating metallic nanoparticle thermal conductivity in fluid. They articulated that the volume fraction of nanoparticles and temperature of the system effects the overall thermal conductivity [8].

Moreover, Cheung carried out research on L-J nanoparticles within solvent and quantified that the detachment energy decreases as the nanoparticle solvent attraction rises [1].

Sun et al. devised a technique using EMD using Green Kubo method to find the effective thermal conductivity of the Cu nanoparticles in Ar liquid. It was found that there was a linear increase in the effective thermal conductivity of shearing nanofluid due to micro-convection [34].

Rudyak and Krasnolutskii later on worked on Aluminium and Lithium nanoparticles with liquid Ar and suggested that the size and material of nanoparticle considerably effects the viscosity [18].

Lin Yun Sheng et al. also detected increment in thermal conductivity by Cu nanoparticle dispersion in Ethylene glycol fluid. In this study, he used Green kubo formulation for finding thermal conductivity using NEMD [35]. Furthermore, Mohebbi investigated a method to calculate thermal conductivity of nanoparticles in fluid using a non-periodic boundary conditions with EMD and NEMD [14].

Kang H et al. carried out work on coupling factor between nanoparticle of Copper and Ar as base fluid, his investigations suggest that coupling factor is proportional to the volume concentration of particles, nevertheless, he also suggested the that there is no effect of temperature change from 90 to 200 K on coupling factor [36].

Rajabpour et al. investigated the specific heat capacity of Cu nanoparticles within water and he found that the specific heat capacity of this system decreases by increasing the volume fraction of particles in base fluid [13].

Loya et al. initiated work on CuO nanoparticles dispersion in water focusing on the change of viscosity due to temperature increase, he figured that temperature increment decreases the viscosity of nanofluid as also initially predicted using experimental testing [37].

In addition to above, further rheological analysis of CuO nanoparticles in straight chain alkanes [28] and water [4] and CeO_2 in water [3] was carried out by Loya et al. For conducting

these simulations, molecular dynamics was used and studies provided highly accurate results of viscosity to experimental findings.

Finally, after knowing the perspective of nanofluid simulation, a simple and general way is deduced for researcher, industrialist and their co-worker in Section 2.3.

2.3. Mimicking different properties of nanofluids using simulation

Several studies about simulation work were reported on the diffusion of polymeric, ionic and mineral nanoparticles [38–40]. An example of this is calcite nanoparticles. These have been simulated in water for salt molecular dynamics for thermal energy storage nanofluidic simulations [38]. Simulations such as these are mostly conceiving diffusions of the polymeric nanoparticles or di-block polymers represented by spheres. The major diffusion phenomena that have been implemented on the nanoparticle or the polymer dispersion is with the help of BD, targeting the random motion of the particles in a solvent or any solution system. Some further surveys show that one of the best simulations for the dispersion of the metal oxide nanoparticle in the water system was carried out using the DPD potential [41–43]. This potential has the power to disperse nanoparticles as well as replicating the phenomena of the BD [44]. DPD was first carried out on nano-water systems by Hooggerbrugge and Koelman [44, 45]. Moreover, the work was carried out by Español and Warren for implementing the DPD technique using statistical mechanics. DPD technique imparts stochastic phenomena on particle dynamics [46]. This is how BD was integrated into DPD technique. However, the random forces will only be in pairwise interaction since DPD at the same time imparts the hydrodynamic effect on the system. Many studies of DPD for complex fluidic systems [41–43] show that the dispersion of nanoparticles in water exhibits complex properties and to simulate this, initial selection of boundary conditions are important to replicate the real scenario. Thereby, the best way to simulate is to acquire the boundary conditions of the existing experimental system and then use a molecular dynamic simulator to further implement it [47]. The considerations of boundary conditions are particle sizes, force field for particle-to-particle interactions, solvent in which the particles will be diffused, and physiochemical nature of the system [48, 49]. Within the simulation system, force field plays an important role since it provides charges on atoms for interaction. The force field is a mathematical parameter that governs the energies and potentials between interactive atoms. The physiochemical settings of the system refer to the thermal, chemical and physical properties of the system such as initial temperature settings, charges and dynamics. Finally, the temperature is controlled using different ensembles.

3. Methodology

3.1. Simulation strategy

The nanofluid interactions are carried out at molecular level. Therefore, by keeping this in mind to conduct nanofluid simulations, it is necessary to have a simulation technique which allows us to do simulation at molecular level. Hence, the technique use for this is molecular

dynamics and package that is focused through this chapter is Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). Furthermore, how to approach this is mentioned in the next section of this chapter i.e. Section 3.1.1.

3.1.1. Approach

The simulation of nanoparticle dispersion is related to the MDS. For this, the software or the package that needs to be selected was based on the criteria of the conditions that were needed to be simulated, and the flexibility was a major concern for the applicability of different systems. The LAMMPS can be a best molecular dynamics package for simulating the nanofluidic system. This is the code generated by the Sandia Laboratories by Plimpton [50]. This molecular dynamics software has high viability over other available software like Montecarlo and Gromacs.

After selection of the MD package, to simulate a desired system with realistic features, it is highly vital to know and understand initial boundary conditions. These initial conditions for a dispersion of nanoparticles are related to charges within the system for interaction, molecular bonding, forces of attraction i.e. Vander Waal or electrostatic coulombs interactions, forcefields, pair potentials (i.e. molecular mechanics constants) and molecular weight. To perform MD simulation, initial boundary conditions are major and fundamental parameters to devise actual dynamics that exist in a real system. After setting the initial parameters, velocity of the system is equilibrated and ensembles are applied to mimic the real thermo-physical conditions.

In addition to above, after setting all the boundary conditions related to chemical and thermophysical parameters, the system is then equilibrated for certain time steps. Simulations are processed until converging results are obtained as that of the actual system. Over here, "time step" is the major dependent factor. This accounts for equilibrating the kinetics of the system that takes place; i.e. movement of system from an un-equilibrated state to equilibrium conditions. The above explained method has been compressed and illustrated using a flowchart for better understanding as shown in **Figure 2**.

After suggesting how to approach and initiate your work for simulation of nanofluids, it is also important to know the briefed-out details about the steps like force field, pair potentials, ensembles, etc.

After setting up the atoms in a coordinate system using a molecular modelling software, then force field is applied on the system (i.e. Universal, COMPASS, OPLS, etc.) by this atomic charges and bond configurations are setup. These force fields are interlinked with pair potentials (such as DPD, BD, Smoothed Particle Hydrodynamic, LJ, etc.), they are parameters which are used to describe vibrational and oscillation settings between two different atoms. Finally, ensembles are applied on the molecular dynamic system for equilibrating the actual thermal settings for example NVT, NPT, NPH, etc.

3.1.2. Techniques and tools

As of now, it is known from the previous sections that to simulate and perform MDS it is necessary to know techniques and tools that can be beneficial for use and executing the work.

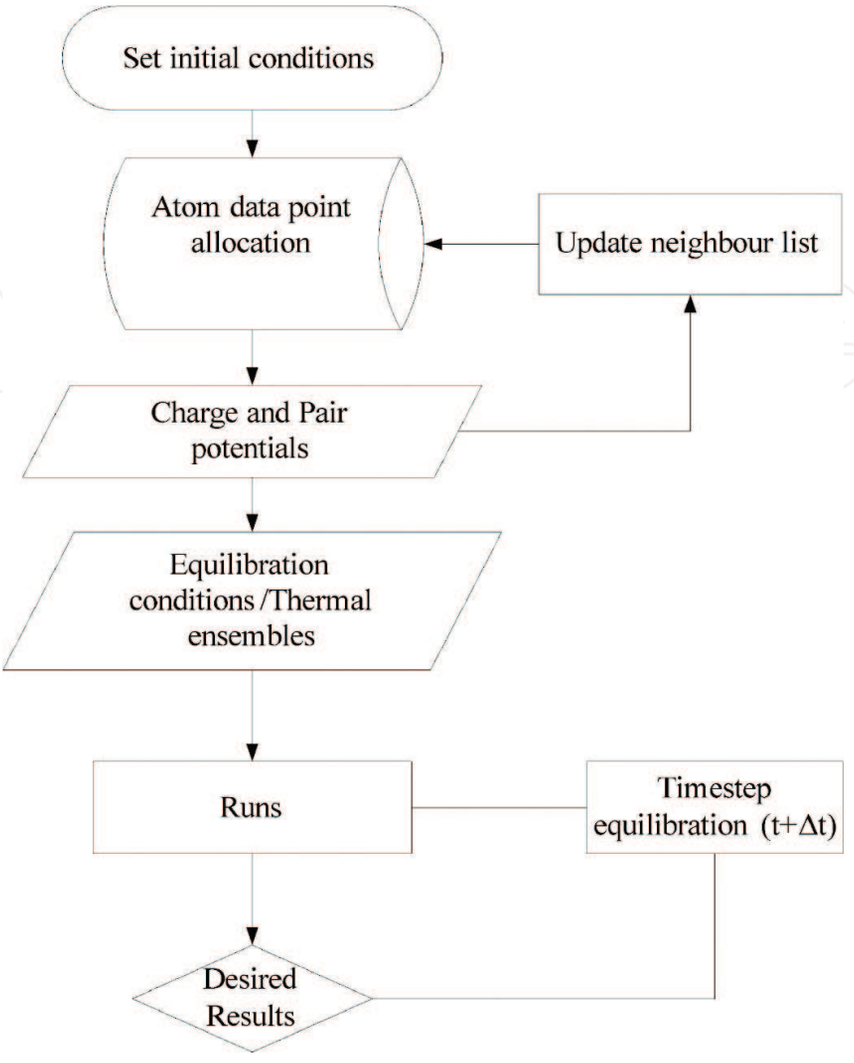

Figure 2. Flow chart of molecular dynamics simulation [26].

Today, there are several tools and ways to perform this; however, still researchers are unsure about "what are the clear steps for conducting nanofluid simulations using molecular dynamics?" Therefore, through this section, a brief and concise way is illustrated and conveyed for better and easier understanding for people working under the horizon of nanofluid simulations. These steps are as follow:

a. Firstly, for creating nanofluid simulation system, it is required to setup a nanoparticle and fluid, then combine them together, for which material studio is the best software for designing a nanoparticle. Now, the nanoparticles can be inserted and replicated in a box containing fluid particles, however, this may be tedious for bigger systems. Therefore, it is suggested to use Packmol after creating the Protein Data Bank (PDB) file from material studio and then create an input script for Packmol to replicate the system with as many particles and fluid molecules as per required. This software automatically packs up the overall molecular arrangement with in a confined imaginary box.

b. As the nanofluid system is set up, now an input data file is required for LAMMPS software, this can be generated by using the PDB file and converting it to required .CAR and .COR format using Material studio. Before conversion do not forget to implement charges on the atoms of the nanoparticle and fluid molecules for this Discover module of the Material studio software can be used. After conversion to .CAR and .COR, use msi2lmp package provided with LAMMPS for converting the file to a LAMMPS readable input.

c. Once the LAMMPS readable input file is generated now use "read data" command for LAMMPS to read this file during the simulation execution.

Finally, the data quantification, visualizing the effects and properties that can be analysed have been jotted below in different sections.

3.1.3. Data quantification

Now, the data obtained by using different compute commands can be quantified on MATLAB or Excel. MATLAB initially requires more time for developing its script for computing the mathematical problem or graphs. However, on a long run, it does save time. Whereas, excel is easy going but requires more time for plotting graph each time you feed the new data.

MATLAB scripting helps in formulating the work in a precise manner, and digitalise the work with high quality publishing of the data for journal publications. However, MATLAB requires good command over the MATLAB scripting and functions. By using MATLAB, it is easy to apply discrete as well as continuous algorithms and equations for refining and optimization of results. Furthermore, it helps in applying the regression on the noisy data for refinement.

In Excel, similar stuff is possible as in MATLAB, but in excel, it is quite complicated as you need to apply macros. These days the computation of MATLAB can be computed in parallel mode; again for excel, it is quite difficult. However, for graphical representation of data, excel is quite versatile.

Vice versa both tools have their own benefits over each other; it depends totally on a user-friendliness with certain software. In addition to excel, to compute or establish complex calculations, it will be required to interlink its macros with visual basic scripting, which is under a developer's tool library, mostly hidden from newbies.

3.1.4. Visualizing the effects

After the successful execution of simulation, you will get dump files from LAMMPS, here a software that can read LAMMPS trajectories can be used for reading the file and visualizing it. For which Visual Molecular Dynamic (VMD) can be used. However, OVITO is also a good software for visualizing your trajectories.

The results generated by OVITO are represented as small spheres merged together to form a particular system representation, as shown in **Figure 3**, i.e. of a CuO-water nanofluid system.

In the similar way for showing how the VMD gives visual output is shown in **Figure 4**. It is similar to that of OVITO, however, VMD has capability of representing the trajectories in the form of molecular structure. This gives an extra possibility for researchers working in the area of Biochemistry, pharmacy, drug delivery and biomedical to represent and observe the chemical kinetics in real-time, i.e. how one atom reacts and interacts with another atom within a confined system.

3.1.5. Properties that can be analysed

Some properties and parameters can directly be analysed using VMD using trajectories dump files. VMD has option for analysing the radial distribution function (RDF) and mean square displacement (MSD), they indicate about the agglomeration and dispersion rate, respectively.

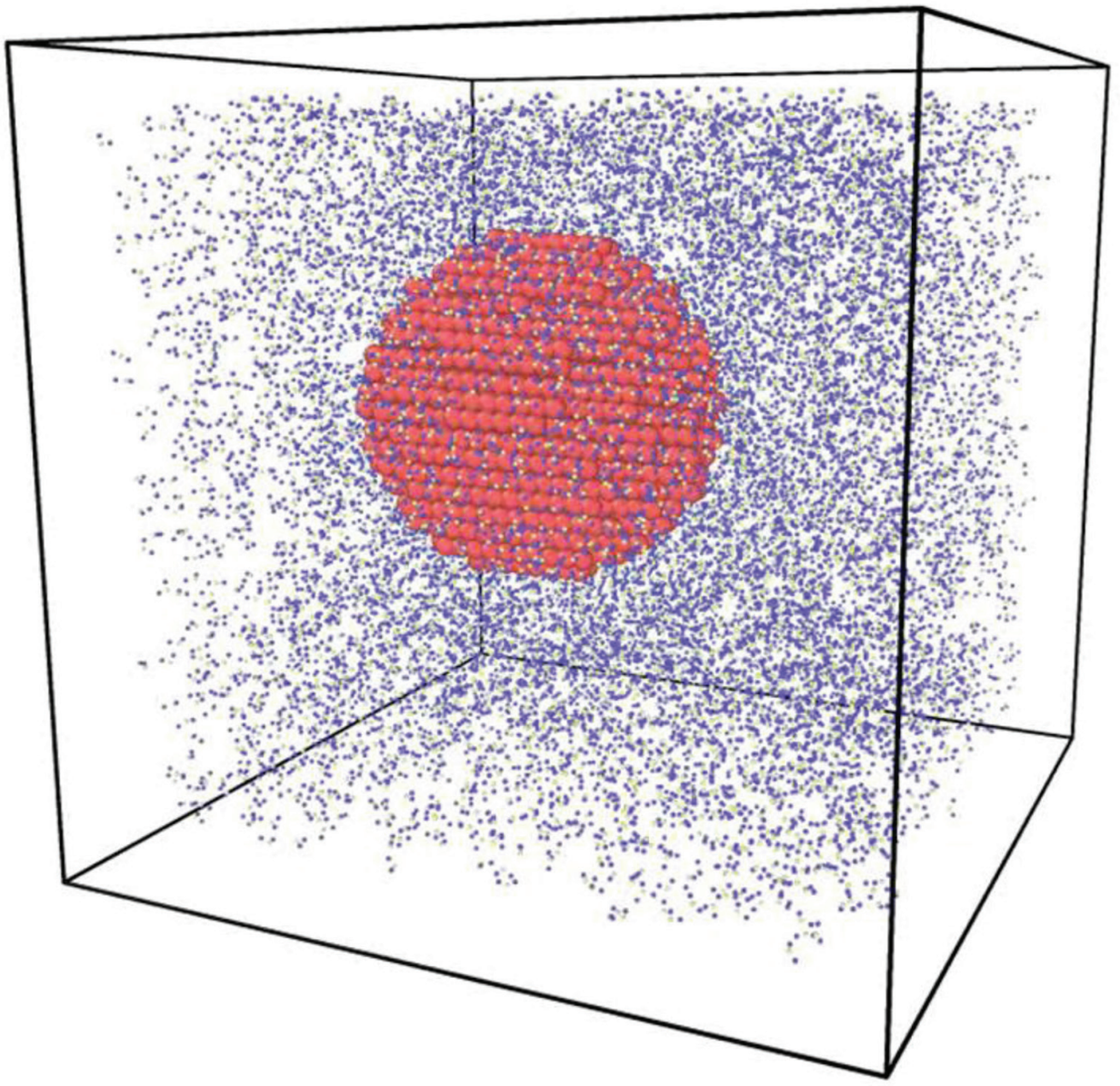

Figure 3. Representation of OVITO output of molecular dynamics of CuO nanoparticles in water system [4].

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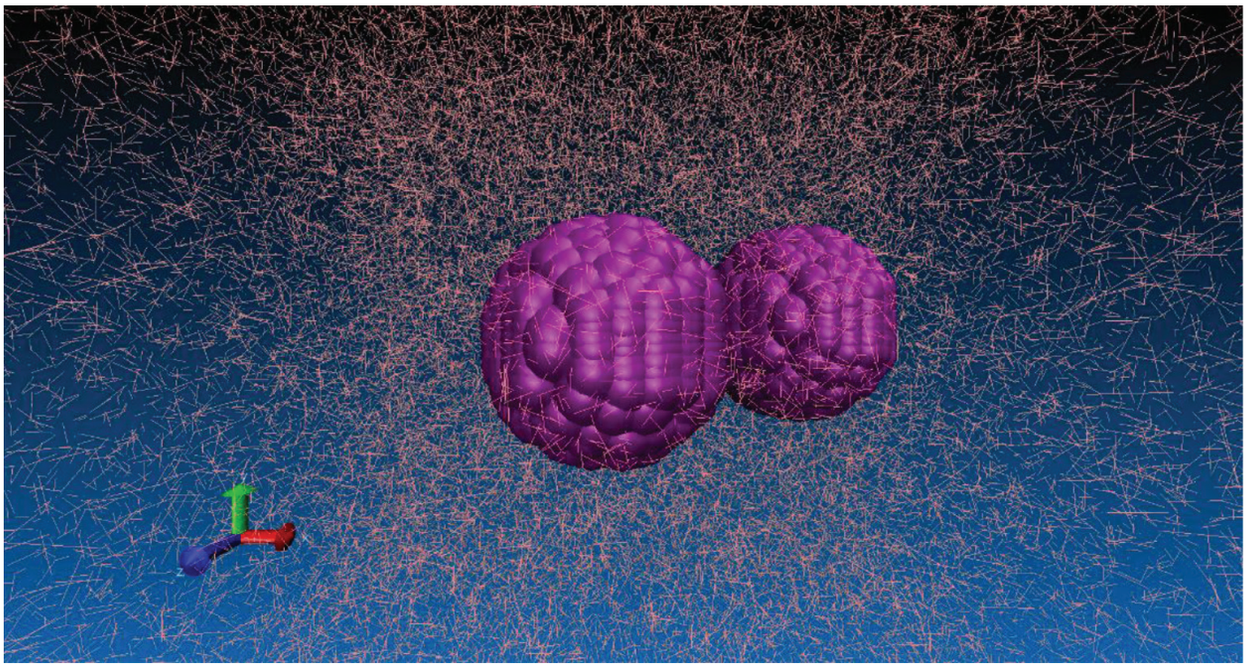

Figure 4. Visual output showing two CuO nanoparticles in a water-based nanofluid.

When nanofluids are concerned the major parameters or properties researcher are interested to investigate are viscosity, thermal conductivity, specific heat capacity, thermal diffusivity, diffusion coefficient, total energy, heat loss, etc. To find these properties LAMMPS provide versatile options to compute what you require, using different algorithms or previously established techniques. Currently, main concerned variables out of above mentioned ones are viscosity, diffusion coefficient and thermal conductivity. Therefore, in the next section, we will discuss about how to validate and quantify your results obtained from the simulation.

4. Validation and quantification of results

To validate the three major properties mentioned in Section 3.1.5, it is required to know initial experimental results, however, sometime it is hard to obtain those results as some simulation condition cannot be tested, either due to lack of experimental device or it is not possible to meet the boundary conditions as setup over the simulation platform.

Now, in this case, the best way is to analyse using autocorrelation function; which is a time series modelling of a function of a variable dependent on time fluctuation. Let us take the case of viscosity, as it is related with shearing stress, there are shear forces acting between the layers of molecular interaction causing pressure function to be induced. This pressure function is dependent on stress due to shearing force. If this stress is analysed using the function of time, this becomes stress tensor. This stress tensor is used for analysing stresses exiting between the molecular layers. Therefore, this is known as stress autocorrelation function (SACF). The SACF accounts for the stresses imparted on the system due to the diffusion of molecules and intermolecular kinetics; i.e. molecular stresses caused by attraction and repulsion of molecules. During the intermolecular kinetics drag is created between the

molecular layers, this drag is due to the effect of shearing forces. Ultimately as the system is equilibrated, it shows unstable response of the SACF, however, as it approaches stability the SACF starts to converge to a monotonic level, which satisfies that the viscosity analysed is acceptable.

In the similar manner, thermal conductivity is quantified, but here instead of stress and shear forces, heat is considered. Therefore, this is known as heat autocorrelation function (HACF), which quantifies or validates the thermal conductivity obtained is satisfactory.

In addition to HACF and SACF for thermal conductivity and viscosity, respectively, for diffusion coefficient, velocity autocorrelation function is used for its quantification. As diffusion coefficient is measured by taking the slope of the MSD. So to quantify and validate it, displacement with respect to time i.e. velocity can be used.

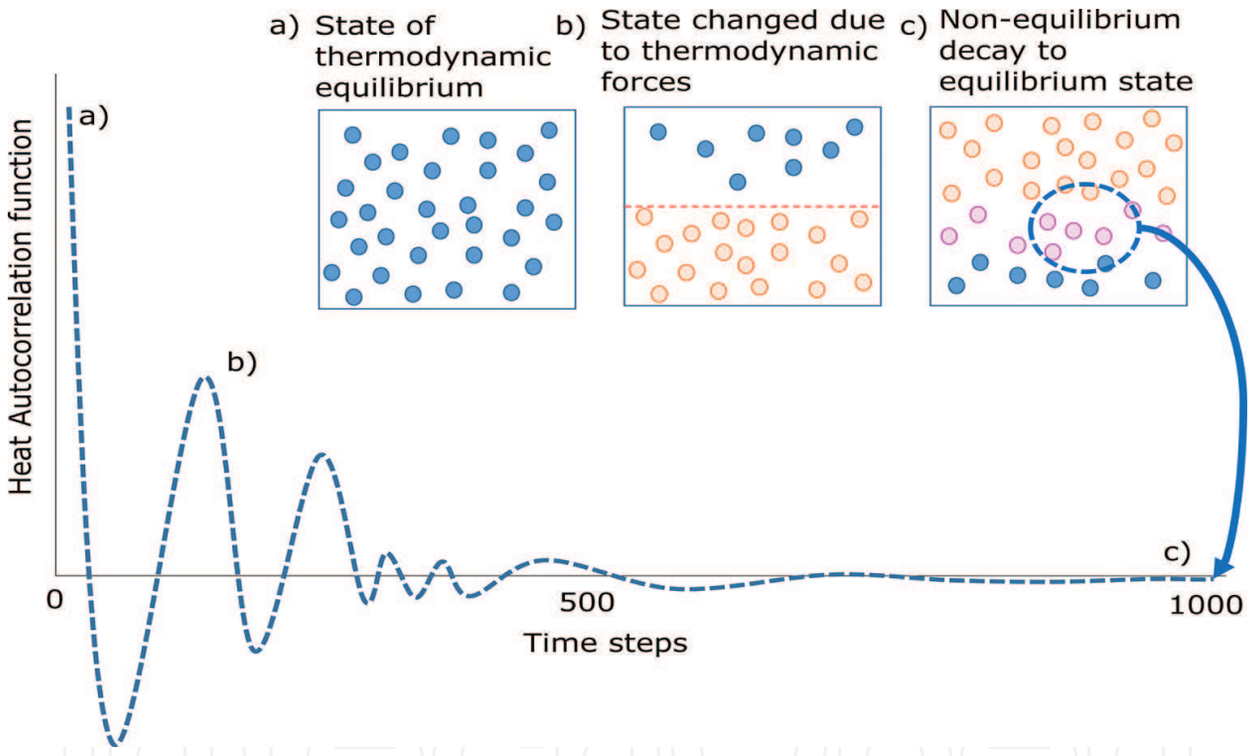

Figure 5. Autocorrelation output gained by running a molecular dynamics simulations [26].

The accuracy of results equilibrated for measuring the viscosity and thermal conductivity of a system can be justified in a better way with the estimation of heat autocorrelation function and stress autocorrelation function as show in **Figure 5**. The graphical result in **Figure 5** explains the process of the integration of non-equilibrated system to equilibration.

At step (a), the system starts with a thermodynamic equilibrium, but the system is not at equilibrium state. At step (b), the thermodynamic conditions are changed due to implementation of thermal ensemble so the system tends to go towards equilibrium. At step (c), the

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non-equilibrium system moves to equilibrated level of convergence at this level the system satisfies the convergences. This process is followed during the equilibration of the thermophysical quantities, the convergence time steps depend on the volume and quantity of the atoms in that system. For the larger system, large amount of computational power and time step will be required for convergence.

5. Discussion

5.1. Problems faced for simulating nanofluids

So far the topic has been conveying the techniques, approach and method for carrying out nanofluid simulations. Moreover, there has been no data available for the expertise to know what are the problems faced when these simulations are conducted, number of questions can arise, for example, (1) Till what level, computational power can support our simulations? (2) Is there any other way out rather than this? (3) How larger systems can be simulated? etc.

Therefore, to answer these questions, it is necessary to understand the material and knowledge given before, however, as the number of atoms are increased within a nanofluid system the molecular dynamics demonstrates sluggish performance due to less computational capabilities i.e. either central processing unit (CPU) power or graphic processing unit (GPU). Furthermore, it is not just simulation that need to be carried out but for the data quantification, the data that are gathered requires huge memory for storage. Thereby, requiring the random access memory (RAM) and hard disk drive (HDD) to be large enough to store the required data easily [51].

After hardware issues, the second set of problems faced by nanofluid simulation is the use of multiple software for designing, modelling, processing and visualization, which needs a lot of understanding of computer for a new geek. Furthermore, if this all is combined in one package, this can marvellously save time and money for purchasing different software for data acquisition. It is slightly known at the moment that there are few software in market for helping in simulating nanofluid; however, academia is not yet aware of it due to less versatility such as Medea and Scienomics MAPS.

One of the major problem is that, people of twenty-first century like working using graphical user interface (GUI), as it is easy and you can do everything by just clicks rather than using complicated commands, however, most of the molecular dynamics package are used on Linux operating system, moreover, commands are used for computing and feeding the data for computation.

In addition to high computing power, it should be known that before attempting to simulate large scale molecular dynamics (i.e. with more than 0.1 million atoms), it is required to have parallel processing enabled on the PC. For that high end, CPU or GPU is required with multi cores for processing the data in parallel mode. However, this processing has some drawbacks that are loop holes for simulations, one such kind is that sometimes the algorithm is not designed in a way to parallel the process efficiently, which in turn gives ambiguous

simulation output and convergence. For avoiding this, it is necessary for the user to know the correct working of the algorithm. Moreover, the field programmable gate array (FPGA) is good outbreak technology that is being implemented for paralleling the process [52, 53], nevertheless, again this technology requires new stuff and bits coding to be learned before operating or using this module for rapidly solving the simulation.

6. Conclusion

The chapter has brought about marvellous information and the literature for new geeks for conducting a nanofluid simulation. However, this chapter acts as a guide for a newbie for initialising the nanofluid simulation.

Nomenclature

Words	**Abbreviation**
Molecular dynamics simulation	MDS
Non-equilibrium molecular dynamics	NEMD
Equilibrium molecular dynamics	EMD
Embedded atom method	EAM
Condensed-phase optimized molecular potentials for atomistic simulation studies	COMPASS
Brownian dynamics	BD
Canonical	**NVT**
Grand canonical	ΔPT
Isobaric and isothermal	NPT
Micro canonical	NVE
Normal pressure hydrocephalus	NPH
Copper oxide	CuO
Titanium oxide	TiO_2
Cerium oxide	CeO_2
Poly ethylene oxide	PEO
Leonard Jones	L-J
Copper	**Cu**
Argon	**Ar**
Kelvin	**K**
Discrete particle dynamics	DPD
Large-scale atomic/molecular massively parallel simulator	LAMMPS
Optimized potential for liquid simulation	sOPLS
Protein Data Bank	PDB
File format output from material studio	CAR and.COR

Visual molecular dynamic	VMD
Radial distribution functions	RDF
Mean square displacement	MSD
Stress autocorrelation function	SACF
Heat autocorrelation function	HACF
Velocity autocorrelation function	VACF
Central processing unit	CPU
Graphic processing unit	GPU
Random access memory	RAM
Hard disk drive	HDD
Graphical user interface	GUI
Field programmable graphic array	FPGA

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