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Integrating Molecular Dynamics Simulation as a Tool for Helping Student Understanding of Fluid Flow Concepts

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Abstract

Molecular dynamics simulation has garnered tremendous attention nowadays as a computational tool to investigate the physical movement and molecular nature of fluids. Molecular dynamics related modeling and visualization software provide a new approach for high school and community college educators to help students understand fluid flow properties. In this study, Research Experience for Teachers (RET) participants developed a set of modules that can be applied at both the high school and college curriculum levels to explore the concepts of fluids (e.g., wetting and spreading kinetics, interfacial thermodynamics, droplet impact, fluid/particle mechanics, etc.) It was the goal of the RET participants to identify best practices for teaching classes such as physics, fluid dynamics, thermodynamics, etc. to explain fluid flow concepts through molecular dynamics simulation.

Introduction

In the broad realm of fluid flow simulations nowadays, a wealth of information has been gleaned from Lattice Boltzmann simulations, phase field and level set descriptions, volume of fluid models, and other boundary tracking schemes of either a sharp or diffuse interface classification. While they cannot resolve macroscopic length and time scales, particle-based simulations, like atomic scale molecular dynamics (MD) methods, possess detail about interfaces and concomitant thermodynamics unavailable to other methods. Molecular dynamics simulations could provide fundamental time and length scale information on atoms. Meanwhile, many properties could be directly computed by MD simulations such as: the extent of spread on surface, dynamic contact angle, flow velocity field, capillary forces, etc.

The most utilized tool in exploring the nuances of fluid flow mechanics is molecular dynamics simulation. Through this utilization, researchers are able to observe simulated response of a fluid through its viscosity, surface tension, droplet movement, and etc. In addition with this simulation software, researchers are able to change the environment of the experiment, by altering its temperature, elemental composition, velocity, and etc. This versatility allows in the discover of the inner workings of fluid flow concepts. However, there is still a significant amount of unknown, thus the importance of continual explorational and utilization of the software. And to that end, it is imperative that younger generations could understand the fluid flow concepts from using MD simulation tools. For this goal, this paper explores the way of incorporating molecular dynamics simulations to convey the different mechanisms of fluid flow concepts. The paper outlines the teaching and learning modules on three fluid flow phenomena through molecular dynamic simulation models and animations via LAMMPS and WOLFRAM MATHEMATICA software.

Course Modules

1. Coffee-ring Effect

The fluid dynamics of pinning occurs within a coffee ring stain. When a drop of coffee is spilled, the boundary that separates the coffee from the air and runs along the surface of the table, all the way around the drop, is called the contact line. Previous research has shown that the edges of a drop evaporate more quickly than the middle. As the edges evaporate, more liquid flows in to take its place. As liquid continues to evaporate from the edges and more flows in from the middle to take its place, coffee particles are being constantly carried to the contact line and left behind. The particles pile up at the edges and stick to the surface, essentially pinning the contact line in place so that the size of the stain doesn't shrink or grow. This creates the thick, dark outline around a coffee stain, which is the "ring" that we see [1].

The coffee-ring pattern originates from the capillary flow induced by the evaporation of the drop: liquid evaporating from the edge is replenished by liquid from the interior. The resulting edgeward flow can carry nearly all the dispersed material to the edge. As a function of time, this process exhibits a "rush-hour" effect, that is, a rapid acceleration of the edgeward flow at the final stage of the drying process.

Evaporation induces a Marangoni flow inside a droplet. The flow, if strong, redistributes particles back to the center of the droplet. Thus, for particles to accumulate at the edges, the liquid must have a weak Marangoni flow, or something must occur to disrupt the flow. For example, surfactants can be added to reduce the liquid's surface tension gradient, disrupting the induced flow. Water has a weak Marangoni flow to begin with, which is then reduced significantly by natural surfactants.

In this coffee-ring effect lab module, students are involved with both experiment and simulation activities. Figure 1 shows the images from class experiment on a coffee drop evaporation, students could observe what happens during the coffee drop evaporation process and finally find out the resulting coffee stain being formed after evaporation. Followed by that is the MD simulation activity. Student will be divided into groups to simulate and animate the evaporation of a coffee droplet via WOLFRAM MATHEMATICA software.

WOLFRAM MATHEMATICA software is designed to create efficient technical computing systems and simulations. It is used to derive a range of studies from complex algebraic equations to algorithmic computations. The versatility of the software has led to its high appeal within industry and education.

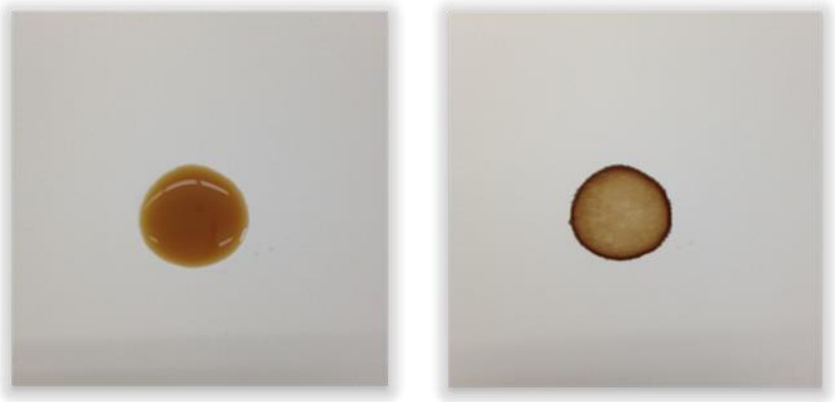

Figure 1: Images from the experiment on a coffee drop evaporation: a drop of wet coffee (left) and the resulting dried stain after evaporation (right).

In the scope of our course modules, The WOLFRAM MATHEMATICA software was chosen for two reasons: the software is capable of producing graphical representations to the user, such as 2D and 3D graphical visualizations, object shape depiction, and real-time image processing. Also, the software is able to import and export visual information of the code, such as images of figures, or video animations of the time-lapses within a graph. A key aspect of MATHEMATICA is its use of built-in functions, enabling the user to simplify their code and eliminate the need to create the functions from the ground up. In addition to the simplicity of the language, it boasts extensive documentation of each function, sharing information about the purpose, parameters, examples of use. With these two focuses, this software was utilized in the development of visual representations of fluid flow mechanics explored in this paper.

Utilizing MATHEMATICA's graphical representation functions, the particles are modeled as circular objects with horizontal and vertical motion. Software facilitates the manipulation and allocation of values to the variables dynamically in real-time. This feature enables the user to precisely observe the reactions occurring in the simulation, and understand the cause and effect of the fluid flow based on the parameters. The manipulation of figures is able to be automated through the software, displaying it as a visual time-based simulation. With the software, the animation can be then exported to an external media file allowing for the universal sharing and viewing of animation. These design steps were applied in the creation of each set of figures below.

In this coffee-ring effect simulation activity, a MATHEMATICA code is developed and shared with students. Each group of students are then assigned to generate simulation figures and videos to observe the entire evaporation process and the direction of Marangoni flow. Meanwhile, they are assigned to change simulation parameters such as droplet and particle sizes and concentration, etc. to examine the resultant influence on the fluid flow process. Figure 2 is an example from this lab activity that shows the simulation snapshots from WOLFRAM MATHEMATICA software that simulates the evaporation of a coffee droplet.

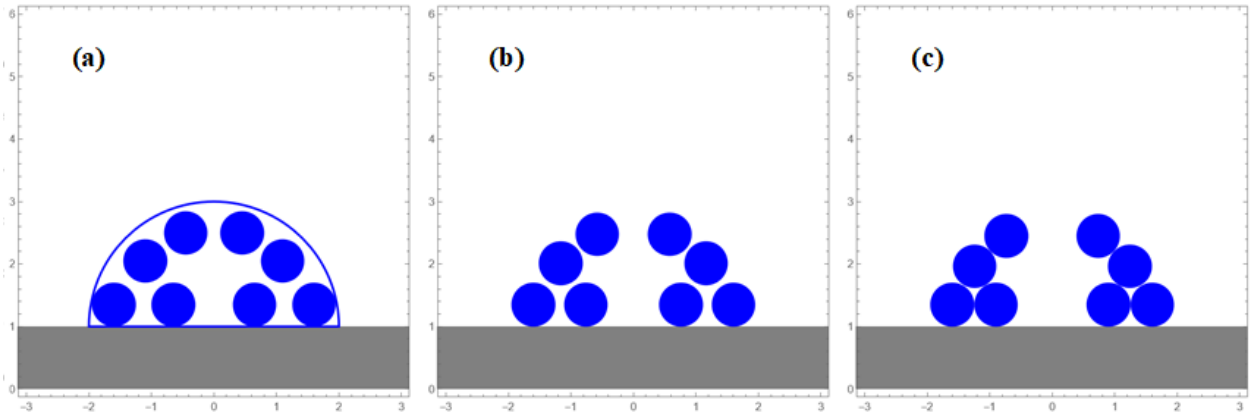

Figure 2: Simulation snapshots from WOLFRAM MATHEMATICA software that simulates the evaporation of a coffee droplet. (a) The initial structure of the droplet before evaporation; (b)

Particles are moving towards the edge of the droplet, due to the Marangoni flow within the droplet; (c) Particles pile up to the edge of the droplet and pin the contact line after evaporation.

2. Droplet Impact on Solid Surfaces

Droplet impact is a constant phenomenon that is integral to the functioning of the natural world. Due to widespread usage in technologies, such as inkjet printers, spray cooling, drug delivery, oil recovery, etc. [2,3,4,5], it's imperative to understand the full capabilities of droplet impact. Thus, there is a wide variety of research towards the interactions between different drops and substrates geared to understanding the behaviors that drops experience. For instance, when a drop collides with a solid substrate, it undergoes one of several different behaviors, such as absorption, bouncing, spreading, and fragmentation. The behavior that had gardened the most interest, is the nuances of drop spreading. Currently, research has concluded that spreading rate is influenced by the droplets size, impact speed, surface tensions, and viscosity [6,7,8]. Even with present findings, there are a multitude of uncertainties surround drop spreading and the varying variables that can altering the spreading rate. These variables are what research are trying to identify and explore the ramifications they produce.

The initial attention to droplet spreading is due to its widespread applications. Drop spreading is a behavior where the droplet impacts a substrate and instead of rebounding or breaking apart, it disperses itself on the substrate. Drop spreading has three stages, and initial, intermediate, and final. The initial stages are defined as a precursors film that moves ahead of the droplet, and the intermediate and final stages are governed by the surface tensions and viscous forces.[9] From observations, it can be concluded that spreading rate can depend on numerous variables, such as impact angle, surface tension of the drop, velocity, electric potential, size, etc. Indicated by other studies, the alteration of theses variable drastically plays a part in the behavior occurring. These variables might affect the speed of nanoparticle spreading, or if the nanoparticle performs one of the other behaviors: fragmentation, bouncing, and absorption.

Students work in groups to investigate the role of impact angle and velocity in dynamic droplet spreading and associated particle positioning on surfaces via using WOLFRAM MATHEMATICA and LAMMPS software (Figure 3 and 4). Then, a class discussion is conducted to provide depth of understanding. Finally, students provide conclusions from what has been discussed and found out from the simulation results.

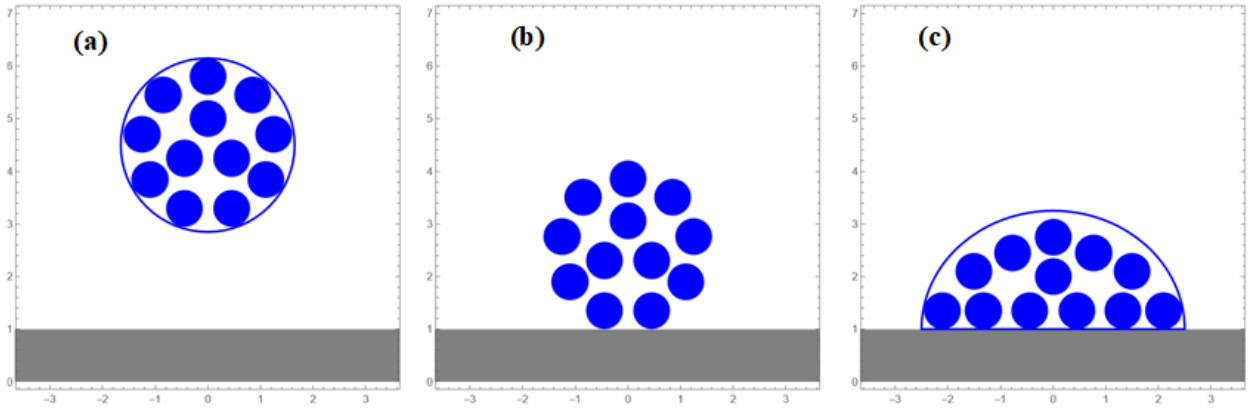

Figure 3: Simulation snapshots from WOLFRAM MATHEMATICA software that show the progression of a droplet impact on a solid surface. (a) the droplet suspends above the gray substrate before impact; (b) the initial impact of the droplet on the substrate; (c) The droplet spreads across the substrate at later stage.

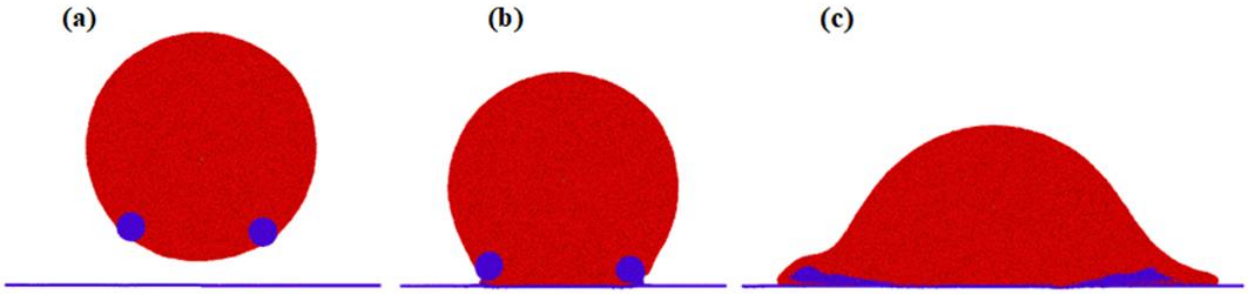

Figure 4: Simulation snapshots of a Pb(l) droplet (red) suspended with two Cu(s) particles (blue) impacting on a Cu(s) substrate from MD code LAMMPS. The impact velocity is 400 m/s and the impact angle is 90 degrees. (a) t = 0 ns; (b) t = 0.065 ns; (c) t = 0.125 ns.

3. Wetting and Spreading Interaction Forces

The process of covering liquids on surfaces is a condition that has found a large range of uses in recent years. From thin film processes such as lens coating to water resistant fabrics, there is an increased need to better understand the processes that allow for the spreading, the flow of a liquid over the surface, and pinning, process of the liquid's resistance to flow as it spreads over a separate medium. These two processes can have a variety of forces that generate them. Among these forces are Van der Waal forces of attraction and repulsion often examined in the Lennard-Jones Standard Potentials. Of greater influence, the forces of adhesion, the attractive forces between liquid and the surface it interacts with, and cohesion, the force of attraction of a liquid to itself, are needed to be examined to identify these processes [10].

There is a lab that developed on simulation of fluid flow interaction forces. Students are assigned notes that they watch virtually. They come to class with these notes completed. These are graded for completion and accuracy. A class discussion ensues to provide context and depth of understanding. Concepts covered include the Rydberg equation, Heisenberg's uncertainty principle, deBroglie's equation, dipole moment, weak and strong forces (Van der Waal & London dispersion forces), and Lennard-Jones potentials.

Students work in groups of two to three on concepts covered. The teacher does an informal assessment to correct misunderstanding and further depth of knowledge.

Students will be divided into three groups (molecular dynamics, LAMMPS, and lattice structure). Students will be given an assignment the night before to read/watch material that they will be responsible to discuss. When they arrive in class, they are assigned questions to discuss and understand as the class experts. They are then assigned to different groups where they provide understanding, and background to the other students in the group as the group expert. They are graded using a rubric, so students have understanding of the expectation for the activity.

Students work with their lab partners through a computer simulation using the pHet simulation from the University of Colorado (see Figure 5). The labs are written into a lab notebook, and questions are assigned and answered. Additionally, students provide a three to five sentence conclusion where they discuss what has been learned and any error they could have made. Lab activity on simulation of Lennard-Jones Potential is provided below and followed by a summative assessment plan.

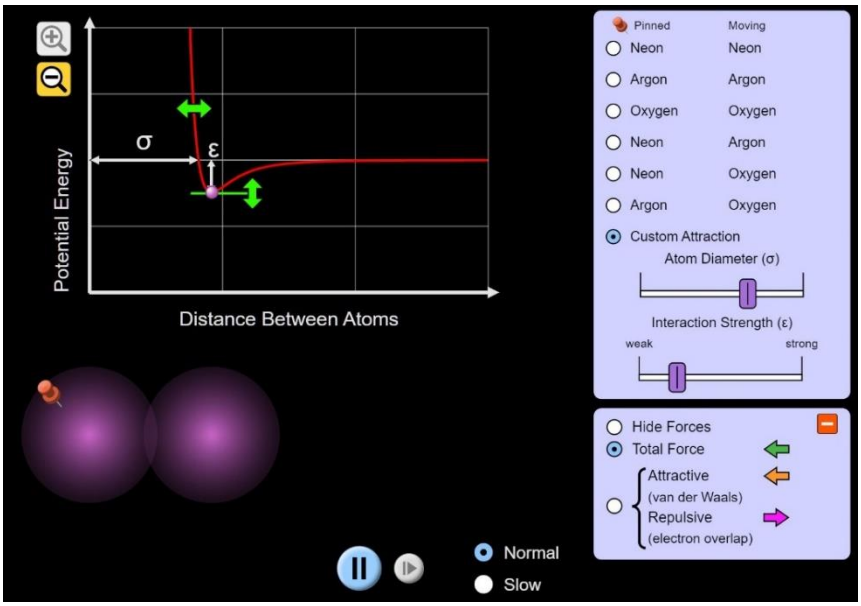

Figure 5: pHet simulation image for describing the interaction forces between atoms.

3.1 Lab Activity

Simulation of Lennard-Jones Potential

Purpose:

This lab is designed as a way of simulating the interaction between atoms much the way that the LAMMPS system does but on a much smaller scale. You will identify the relationship between energy and distance based on the various atoms provided.

Procedure:

1. You and your partner will take your iPads and log on to the pHet simulation.
2. Assume each line on the x-axis represents 1 angstrom (Å). Assume each line on the y-axis represents 10 kJ/mole. You will need to make approximations so do the best that you can.
3. In the data table, list the atoms interacting and the approximate length and energy for each interaction.
4. If you need to do so, adjust the scale by pressing the negative magnifying glass on the left of the graph.

5. After you have gone through all the set atomic interactions, click on the custom attraction and move the atom distance to the minimum position, and the interaction strength to the maximum.
6. Record your values for length and energy in your data table below.
7. Repeat steps 5 & 6 with values equal and reversed. (Atom distance at a maximum & interaction strength at a minimum.)
8. Once you have completed this, shut down the simulation, and answer the questions with your lab partner.

Questions:

1. Identify 2 factors about the pre-set interactions that you can identify, and how these could play a role in the interactions that you observed.
2. What relationship did you observe as you ran through the customization steps in the lab? (Steps 5 - 7)
3. Identify an advantaged, and possible disadvantage that the simulation could present as opposed to operating in macro (or real-world interactions.)

Trials	1st Atom	2nd Atom	Approx. Length	Approx. Energy
1				
2				
3				
4				
5				
6				
Distance Min vs Strength Max				
Equal Values				
Distance Max vs				

Strength Min				

3.2 Summative Assessment Plan

Quiz:

Biweekly, students are assigned a Google Form quiz as to the material covered in the class over the past two weeks. The quiz is assigned at the start of class on a practice day. This will give some evaluation of where the student's understanding is and where modifications and corrections need to be made for instruction.

Unit Test:

At the completion of the unit, a test will be given. It will contain both verbal and mathematical problems. The verbal section will be a combination of multiple select, matching, true/false, and an essay question. The mathematical section will contain problems from the section that will demonstrate the student's understanding of the concepts presented. These are partial credit problems that range from five to thirty-five points in value. Students will have the opportunity to obtain as many of these points as possible by showing all appropriate work. Points are assigned for each step of the process as well as three final points for the answer for the correct answer, the correct units, and the correct number of significant figures in the answer.

Conclusion

In this study, Research Experience for Teachers (RET) participants developed three course modules that can be applied at both the high school and college curriculum levels to explore the concepts of fluids via Molecular Dynamics Simulations. Related lab activities and assessment plan are provided in detail. Student learning is enhanced with the interactive simulation modules according to the course assessment results and feedback from students. In the future study, we plan to create new educational materials to aid the teaching of fluid flow subjects and even more broad STEM related subjects.