Numerical Algorithms Applied to Computational Quantum Chemistry

Simulating Water Freezing Using Canonical Ensembles (NVT)

Link to Main Github Repo: https://github.com/dturk0610/CHEM279_Final_Project/tree/main
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Dakota's Github Submission: https://github.com/dturk0610/CHEM279_Fall2024_dturk0610
Matt's Github Submission:

Abstract

The focus of this project was the development of a user-focused simulation of water behavior under Canonical Ensemble (NVT) conditions, featuring an interactive graphical user interface (GUI) accessible via a web page. The simulation aimed to improve upon existing industry-standard water models, specifically TIP3P and SPC/E, by implementing a hybrid approach that combined Lennard-Jones (van der Waals) and Coulombic force calculations derived from both models. This hybrid framework modeled water's thermodynamic behavior, capturing energy minimization and force stabilization trends as the system approached near-zero temperatures.

The results show a gradual decrease in potential energy, stabilizing near -24.0 kJ/mol, which closely aligns with literature values for the TIP3P and SPC/E models, despite computational limitations and the primitive nature of the current model. This project highlights the utility of blending theoretical approaches while prioritizing usability, addressing a key limitation of existing studies that lack accessible, educational visual interfaces. The current simulation successfully models basic properties of water, but remains rudimentary compared to the team's original vision of simulating phase transitions. Future developments will focus on implementing additional physical properties and creating a modular framework with plugin capabilities to enhance adaptability and further development.

Introduction

The molecular simulation of water is critical to enhancing our understanding of its unique properties, which underpin its significance in numerous scientific applications. Water (H_2O), comprising two hydrogen atoms covalently bonded to one oxygen atom, possesses a bent geometry due to the lone electron pairs on the oxygen atom. This geometry gives water a pronounced dipole moment, featuring partial negative and positive charges localized on the oxygen and hydrogen atoms, respectively. Water's polarity and hydrogen bonding abilities result in anomalous physical and chemical properties, such as its high dielectric constant and cohesion. These properties are central to its roles in biological systems, materials science, and energy research.

Despite the breadth of experimental studies documenting water's properties, such methods often pose constraints in terms of cost, time, user interface and scalability for modern applications. Computational approaches with visual components, such as molecular dynamics (MD) simulations, offer a powerful alternative by modeling water's behavior at the molecular level. For example, accurate water simulations are pivotal in drug discovery, where protein-ligand interactions are modeled via tools like Alphabet inc. AlphaFold requires validation in aqueous environments to assess a drug candidate's viability (Abramson, 2024). Similarly, water simulations play a key role in optimizing materials and processes in fields such as nuclear research and renewable energy.

Various structural models of water have been developed to capture its molecular and intermolecular interactions. Among the most widely used are the Simple Point Charge (SPC) model and its extended version, SPC/E. These models treat water as a rigid molecule with charges positioned at the oxygen and hydrogen atoms, albeit with parameter variations to refine charge distributions (Water models, 2001). The Transferable Intermolecular Potential with 3 Points (TIP3P) model, commonly used for biomolecular simulations, introduces Lennard-Jones parameters to enhance accuracy by capturing short-range interactions at all atomic sites. Polarizable models, such as POL3, further improve accuracy by allowing dynamic polarization and flexibility of the molecular geometry. However, these approaches come with increased computational costs. While SPC and TIP3P are computationally efficient for general-purpose or biological simulations, polarizable models offer superior accuracy for hydrogen bonding and electrostatic interactions, albeit at the expense of higher computational demands.

The thermodynamic conditions under which simulations are conducted are equally critical. MD simulations typically use statistical ensembles to model physical systems under specific constraints. For instance, the microcanonical ensemble (NVE) maintains a constant number of particles (N), volume (V), and total energy (E) but is less suited for systems requiring constant temperature or pressure (Libretexts, 2022). The canonical ensemble (NVT), by contrast, allows thermal equilibration via thermostats to maintain constant temperature, ensuring realistic temperature fluctuations that mimic experimental conditions.

This project aims to build a foundational simulation framework using a hybrid structural model that combines the simplicity of SPC with the parametric accuracy of TIP3P supplemented with a graphical user interface for broader scientific accessibility. The simulation is conducted under NVT ensemble conditions, ensuring constant temperature, volume, and particle number, while incorporating gradual cooling to simulate hydrogen bonding and crystallization processes. A basic thermostat is implemented at the simulation boundaries to maintain thermal equilibrium

and enable energy fluctuations resembling real-world scenarios. By exploring the freezing process of water, this study provides insights into the molecular dynamics of crystallization and contributes to the development of realistic water models for applications across various scientific fields.

Methods

Theoretical Approach

The energy of the system was calculated using a hybrid SPC and TIP3P structural model, which mainly focused on the oxygen-oxygen interactions for simplicity. These models consider two major intermolecular forces: Van der Waals interactions (modeled using the Lennard-Jones potential) and Coulombic interactions (accounting for electrostatic forces between partial charges). The total potential energy U_{total} a system is expressed as the sum of the Lennard-Jones potential and Coulombic potentials over all pairs of interacting molecules. Therefore, since the two potentials that were considered in the SPC and TIP3P model were the Lennard Jones potential and the Coulombic. The total potential energy of the system would be:

$$U_{total} = \sum_{i<j} [U_{LJ}(r_{ij}) + U_{Coulomb}(r_{ij})]$$

equation 1.

Lennard-Jones Potential:

Then to calculate the Lennard Jones, which represents the van der Waals forces prevalent in molecular behavior the following 12-6 variation:

$$U_{LJ}(r_{OO}) = 4\varepsilon_{SPC}[(\frac{\sigma_{SPC/E}}{r_{OO}})^{12} - (\frac{\sigma_{SPC/E}}{r_{OO}})^{6}]$$

equation 2.

Where r_{OO} represents the distance between the two oxygen atoms of two water molecules. The σ symbol is the finite distance at which the interparticle potential is zero, and ϵ is the depth of the potential well (an energy constant) of the theoretical approach. This equation highlights the balance between the repulsive (12th power term) and the attractive (6th power term) forces. The Coulombic interaction $U_{coulombic}$ represents the electrostatic forces between the partial charges on hydrogen and oxygen atoms which are given by:

$$U_{Coulomb}(r_{ij}) = \frac{1}{4\pi\varepsilon_0}\frac{q_i q_j}{r_{ij}}$$

equation 3.

Where q_i and q_j are the partial charges on corresponding atoms, r_{ij} is the distance between atoms i and j, and ε_0 is the vacuum permittivity constant. The forces acting on the molecules are calculated as the negative gradient of the potential energies. Specifically for Lennard-Jones interactions the force between two oxygen atom is given as

$$\vec{F}_{\text{LJ}}(r) = -\nabla V_{\text{LJ}}(r) = 24\varepsilon \left[2 \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \frac{\vec{r}}{r^2}$$

equation 4.

Similarly, coulombic forces are computed for each interacting pair of atoms contributing to the overall dynamics of the system.

Computational Approach

To simulate the system, a canonical ensemble(NVT) approach was implemented, to ensure a simulation of water under a gradual decrease in cooling conditions. Combining the above molecular dynamics calculations with a canonical (NVT) ensemble the simulation was successfully modeled. This framework ensures the number of particles (N), volume(V), and temperature(T) remain constant. To complete the objective set forth, a basic thermostat that was developed through use of velocity Verlet algorithm to maintain the target average temperature constant by incrementally decreasing the instantaneous temperature anytime a molecule interacted with the boundaries of the box. The simulation proceeded with a set of six different stages:

Initial configuration:

The water molecules are initialized in a cubic grid, with positions and velocities assigned based on the Maxwell-Boltzman distribution at the desired starting temperature based on user input. The velocities are scaled to match the kinetic energy derived from the system temperature using the following:

$$KE_{\text{total}} = \sum_{i=1}^{N} \frac{1}{2} m_i \left(v_{i,x}^2 + v_{i,y}^2 + v_{i,z}^2 \right)$$

equation 5.

The positions and orientations of the water molecules are initialized with random small perturbations to prevent uniformity and molecular overlap.

Force calculations:

Next, force calculations are done at each timestep, the forces between water molecules are computed using the Lennard Jones and Coulombic potentials. The coulombic forces are computed for partial charges on oxygen and hydrogen atoms while the Lennard Jones forces are determined for oxygen-oxygen interactions only. This was done due to the mass of oxygen compared to hydrogens, and an approach taken by the SPC method to simplify water-water molecular interaction at oxygen level. The positions and velocities are updated using the velocity Verlet algorithm for time integration:

$$\vec{r}(t + \Delta t) = \vec{r}(t) + \vec{v}(t)\Delta t + \frac{1}{2}\vec{a}(t)\Delta t^2$$

equation 6.

$$\vec{v}(t + \Delta t) = \vec{v}(t) + \frac{1}{2}\left[\vec{a}(t) + \vec{a}(t + \Delta t)\right]\Delta t$$

<div align="right">equation 7.</div>

The acceleration a_i is determined by the forces acting on each molecule as:

$$\vec{a}_i = \frac{\vec{F}_i}{m_i}$$

<div align="right">equation 8.</div>

The velocity rescaling thermostat is applied at each step to maintain the target temperature. The velocities of the molecules are adjusted when they interact with the boundaries; this approach although, very basic, ensures system temperature remains stable while allowing for natural fluctuations. Therefore, simulation can incorporate the process of gradual cooling incrementally mimicking real world cooling conditions. Lastly, the metrics such as the total potential energy, kinetic energy, coulombic forces, angular torque forced due to hydrogen-hydrogen repulsions causing the oxygen atom of the water molecule to spin. These rotations were all recorded at each timestep to analyze the system's dynamics in terms of torque. Energy distribution and hydrogen bonding patterns are monitored to observe possible transition from liquid and natural nucleation taking place.

For simulation input parameters, we aimed to allow the user to choose the initial amount of particles and the initial temperature of the system. This means we are keeping the volume and pressure in the system constant overtime. However, due to time constraints, the system was mostly only tested with no change in temperature and the particles only interacting with each other. While the simulation will run with the temperature value changed, it does cause some bugs to pop up during the calculations where particles begin to overlap, causing NaN values to appear in the code and effectively causing many of the particles to just blip out of existence. This is something that will be looked at as the project progresses and hopefully will be resolved in the near future.

Software Stack

The software stack for this project was designed as a backend, server and client. With the focus around the user needing to do as little as possible in order to visualize the water particles. With this in mind, our project is completely contained inside of a Docker container and uses HTML for visualization. This allows our system to be run on nearly any machine, and if the network setup is correct, allows the user to pull the simulation up on any device within their local network.
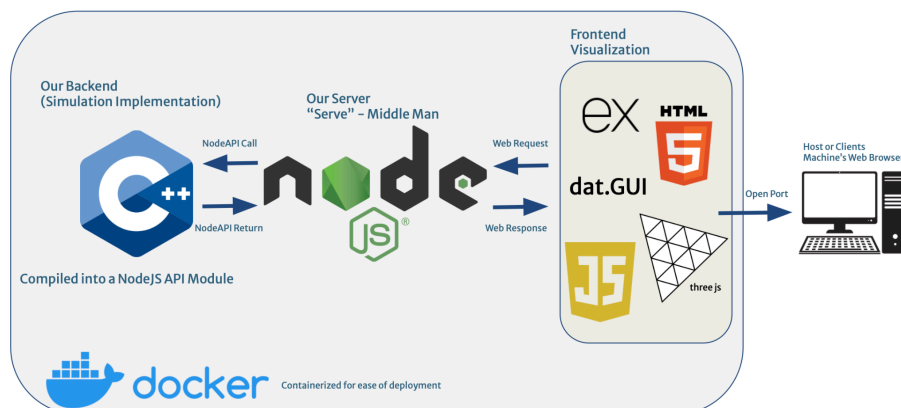
The client is implemented using entirely HTML and javascript. This is done through a series of widely available and used packages like ThreeJS and dat.GUI. The aim with the client code is simply to receive information from the server in the form of condensed web packets. More about this will be in the backend portion of the stack. This code starts by preparing the GUI and simulation for preparing to run.

The server portion of the stack is implemented using NodeJS. In this case the server's role is to serve packets from the client to the backend, then serve the responses from the backend over to the client again. There is not much else happening in the server scripts as they are designed to be as lightweight as possible. It is important to note here that the server code is able to import the compiled custom NodeJS module, which is the backend end code.

The backend code is where the actual simulation lives. This code is split into the simulation portion, then the API layer which is what is called by the NodeJS code. In order to send the information from the simulation over to the server, we pack the data into one single large byte array. Since we are communicating to the client each point's position, velocity, rotation and bond angle which are all stored as float values, we are creating a very large byte array that is getting sent. The positions are a 3xN, velocities a 3xN, rotations a 4xN and bond angles of size N arrays, where N is the number of particles in the system. Each of these arrays are flattened and then stack together to make the buffer array that gets sent to the server and then ultimately the client. Where the data gets unpacked and rendered.

The aim here was to make the simulation modular such that much of the code is functionalized, so that it is easy to add or remove new force calculations and implement them into the code. Due to the Velocity-Verlet algorithm, the only thing one would need to do in order to have the simulation run is to update the force values after each time they are initialized back to zero at the start of each frame. There are still many things that could be done to improve the simulation speed, such as parallelization. More of this will be discussed, further in the future development section.
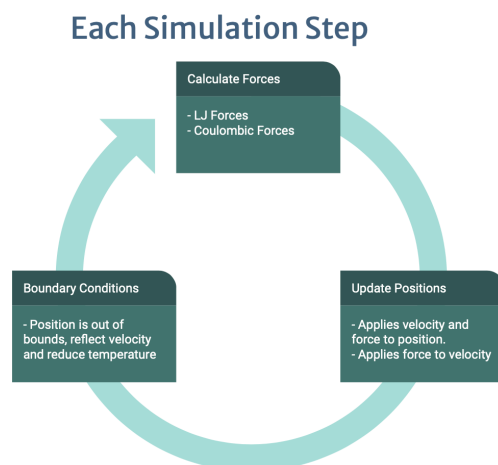
Results

       In this project the average potential energy, forces and torque for a system of water molecules were evaluated using the hybrid model described earlier. The results provide insights into the behavior of water molecules over time under specific simulation conditions and highlights a comparison with other simulation models.

       The potential energy of the system was monitored over time as shown in *figures one* and *two*. Figure one depicts the average energy between just two water molecules, hence the extreme oscillatory changes. Figure two shows the same average energy over time for 53 molecules, where there is a smoother noticeable decrease in energy. The two comparisons were made to test the simulation's ability to track energy of the system in extreme conditions, within the computational resources the team had available.

       The Lennard-Jones (LJ) potential energy, which represents the van der Waals interactions between oxygen atoms, shows a clear decreasing trend, indicating that stabilization of the system as temperature decreases. In the initial stages the energy exhibits a significant fluctuation because of higher kinetic energy and unoptimized molecular arrangements randomly set. Overtime, the average energy decreases with molecular interactions via the boundaries, and eventually stabilizes molecule interactions aligning with theoretical expectations as the system approaches low temperature conditions. The final energy values stabilizes near $-4.0 \times 10^{-20} J$ (-24.0 kJ/mol or -5 kcal/mol), consistent with the theoretical predictions and reported results for water models such as the TIP3P and SPC/E in previous research(Jorgensen et al., 1983; Berendsen et al., 1987).

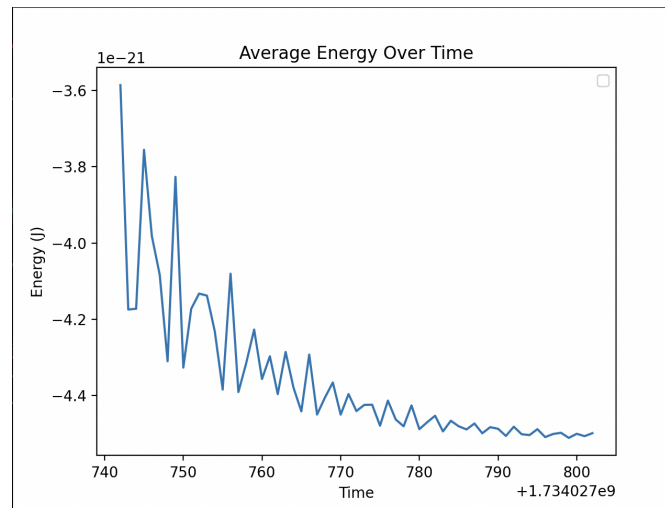## Figure 1: Average Energy of Two Water Molecules

Figure 1: (granular) indicates more granular fluctuations which smothens as the system reaches lower temperatures. This behavior is typical for energy minimization in MD simulations.

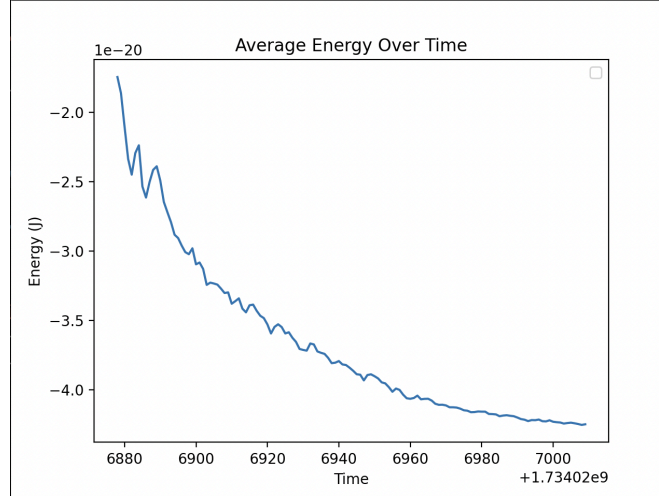## Figure 2: Average Energy of Fifty-Three Water Molecules

Figure 2: (general) this shows the average energy stabilizes near $-4.0 \times 10^{-20} J \, or \, -24.0 \, kJ/mol$, consistent with the reported energy values of water models TIP3P and SPC/E.

The forces and torques acting on the water molecules were analyzed, as shown in figure *three*. The force contributions were further broken down into LJ-forces(fLJ), coulombic forces (fC) and torque values (tv). The LJ forces gradually decrease over time aligning with the observed reduction in system energy stabilization of molecular arrangements. This trend confirms the role of van der Waals interactions in driving the system toward a lower-energy state. The Coulombic forces show minor fluctuations, but remain stable, reflecting the balance of the electrostatic forces as partial charges on the oxygen and hydrogen atom interactions. The torque values remain consistent with molecular reorientation processes as the system evolves.
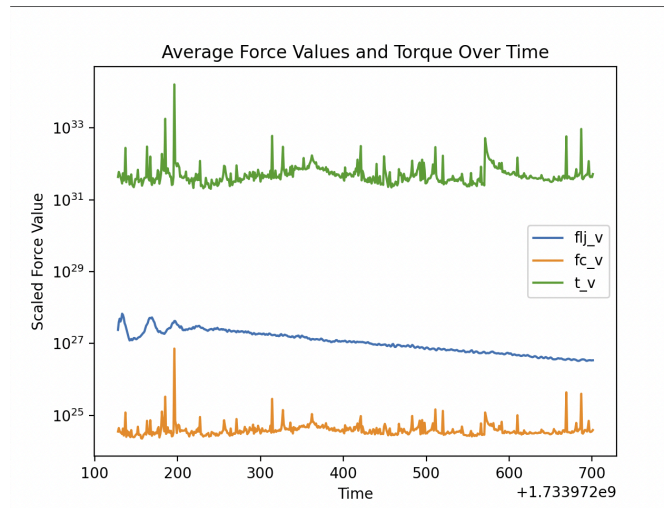
Figure 3: Average Force and Torque Values

Figure 3: The Lennard Jones forces gradually decrease, correlating with the reduction in system energy overtime. Lennard-Jones forces (f_{LJ}), Coulombic forces (f_c), Torque values (t_v).

The results above align well with the reported behavior of widely used water models such as TIP3P and SPC/E as expected. According to Jorgensen et al. (1983) and Berendensen et al. (1987), the average potential energy of liquid water systems stabilized at approximately -40 kJ/mol at 300 Kelvin, here our model got -24KJ/mol at 0K ($-4.0 \times 10^{-20} J$) under close to similar density and temperature conditions *(appendix table 1)*. Lastly, the fluctuations observed in the force and energy profiles during the initial stages of the simulation is consistent with MD simulation behavior of high initial kinetic energy caused by rapid oscillations of the molecules. The LJ forces and coulombic interactions both show a decreasing trend towards the end of the simulation indicating an overall stabilization of the system as originally hypothesized.

<u>Discussion</u>

The development of this project demonstrates the potential effectiveness of using a hybrid SPC model that combines Lennard Jones and Coulombic forces to simulate the behavior of water under NVT conditions. The modular aspect of the code enables further development of the simulation by adding additional factors to the existing framework. By monitoring the potential energy, forces and torques in the system the model captures the stabilization behavior of water molecules as the temperature decreases. The results, particularly the minimization observed in *figure one* and *two*, validate the accuracy of this approach. Although the existing simulation is a crude hybrid version of the fundamental concepts underlying the SPC/E and TIP3P model, it still manages to closely achieve similar results. Thus, highlighting the potential capability of the model to further develop into a more complex and highly efficient simulation.

The decreasing trend in Lennard Jones forces and the corresponding reduction in system energy highlights the utility of incorporating the van der Waals and electrostatic interactions for modeling water behavior. The stabilization of energy near $-4.0 \times 10^{-20} J$ aligns closely with the literature reported values for SPC/E simulations((Jorgensen et al., 1983; Berendsen et al., 1987), indicating the robustness of the hybrid model despite its crude development. However, the results also reveal some limitations of the current implementation. For example, the initial fluctuations in energy and force values as seen in *figure three*, stem from unoptimized molecular configuration and high initial kinetic energy.

This can be optimized with alternative statistca distribution methods by A/B testing various random distributions to minimize this behavior. Additionally, the simulation provides only short term behavior, for a limited small number of molecules which in practical research may not be feasible. Thus, further development of the program performance is pivotal for large computations.

Lastly, in order to fully observe the initial objective envisioned when this project was initialized, bond angle optimization along with nucleation must be considered within near zero temperatures. This can be done through implementation of a framework similar to Höllmer et al. Where an algorithm is developed in conjunction with monte carlo simulation to optimize bond angles in accordance to Lennard Jones potentials (Höllmer, 2024). A similar framework added to existing simulation can significantly increase the utilization of this simulation and bring about insights into water phase change at a computational level. Nonetheless, it should be noted that the objective of this project was to develop the simulation with a visualization and user

experience in mind as the core responsibility of the team. This was successfully achieved with a aforementioned software development stack.

Future Development

Currently, all of the code runs on a single thread. A massive optimization that could happen relatively quickly would be to parallelize the code such that the simulation steps can be broken down into more efficient segments that can be highly optimized for parallelization. This would drastically reduce the amount of time that the simulation code takes to compute incredibly large particle count amounts.

The developed code obviously lacks many properties of water and has massive potential for being expanded. In this section potential and probable future development of the system. During development, one issue that stood out among the rest was the problem of unit conversion. One improvement that would set this system out among the rest would be to create a unit checking system that allows users to input their units for their equations and allow for auto error detection and possible correction.

Adding in more properties for water that would also prove to make the simulation more accurate. Things like thermal expansion, isobaric heat capacity and dielectric constants. All of these would greatly improve the accuracy of the water simulation itself, while likely having a big impact on the performance of the calculations.

Throughout the development, the team also discussed the possibility of adding in Monte Carlo based determinations of bond angles for the atoms, so that a more natural progression of bond angles could be simulated(Höllmer). Unfortunately, in the final product, the system keeps a strict bond angle size which is where we could likely be seeing a current negative impact on our current iteration of the simulation.

Finally, the most impactful change to the system would be to implement a large-scale modularization framework that could work with plugins developed by anyone to allow for a highly adaptable and scalable system. This kind of system would take time to implement, but is a necessary evil so that the simulation could be used to visualize the interactions of particles much easier. A first approach would be to first create an API system that would allow for changing any force calculation into the system. After that would need to be positional updates for the molecules. A couple final steps would then be to make the molecule object itself highly modular where the user could potentially provide their own object in order to model their exact needs.

Final Thoughts

While the system that was implemented was originally to try and re-create a much more basic water simulation, this project has grown a great deal away from that original scope. LJ forces were able to be accurately implemented and working with relative ease. Similarly, the bounds checking and velocity-verlet equations. All of which our team were able to pull in from other courses that we have taken during our time in the MSSE program. We were able to approach this problem with relative ease and efficiency due to the equation and algorithm implementations that we have learned throughout this course. Even being able to pull in the docker containerized environment and efficiencies that we learned in the CHEM281 course.

Ultimately, this was a very ambitious project for our team to take on, and while we still plan to further it even more and allow for other types of energy calculations, the team was very happy and satisfied even with the current results that we have. Yes, there are still some minor bugs in the code and handling of the rotations/torques of the molecules. However, our team is very confident that if given more time, these bugs would be able to be resolved with relative ease. After expanding the system to a more modular one, individuals would be able to create custom packages that could pull in components from LAMPS or other MD software packages that use significantly more accurate calculations.

This projects presents a novel approach to how MD simulations could easily be implemented to create more visual environments that would allow for much faster interpretations of how specific energy calculations can affect a system and could easily assist in real-time understanding of many types of chemical reactions or other processes like protein binding with drug discovery or other topics like previously.

The visuals will be of great substance when visualizing protein structure docking into ligand binding domain with presence of water molecules. This detailed visual would enable chemists to better understand how to optimize ligand and protein structure in the context of drug discovery.Therefore, our team believes that this project could serve as a very good springboard for other's work or research. Especially when considering that many simulations are typically resolved by printing out large sheets of data that is only afterwards passed into visualization software like VMD. This project acts as a starting point to visually understand how these kinds of simulations expand or resolve over time and would assist greatly in the education field for newcomers to see the impact of their work and studies.

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Appendix

1. Benchmark results for TIP/3P Water model

Table 1. SPC/E model Potential Energy Berendsen et al.

TABLE I: Simulations on Polarization-Corrected SPC:Water[a]

model	SPC[b]	1	2	3	4 = SPC/E	exptl
q_H	0.41	0.437	0.422	0.427	0.4238	
B	0.3428	0.34505	0.343	0.3431	0.3428	
$\mu/10^{-30}$ C m	7.585	8.085	7.807	7.900	7.841	6.171 (vac)
μ/D	2.274	2.424	2.341	2.368	2.351	1.85 (vac)
E_{pol}	3.74	6.86	5.01	5.60	5.22	
MD run/ps	20	15	17.5	17.75	27.5	
E_{pot}	−37.7	−42.0	−40.6	−41.9	−41.4	−41.5[c]
T/K	308	306	307	305	306	
press./bar	−1	4	6	9	6	
density/ g·cm^{-3}	0.970	0.981	0.992	0.994	0.998	0.995 (305 K)
diff const	4.3	(2.7)	2.9	2.2	2.5	2.4 (300 K) 2.7 (305 K)
$\partial E_{pot}/\partial q_H$	−236	−271	−259	−266	−262	
$\partial E_{pot}/\partial B$	754	875	835	864	850	
$\partial p/\partial q_H$	−7.9		−8.9	−9.1	−9.1	
$\partial p/\partial B$	8.2		9.2	9.5	9.4	

[a] Units (if not specified): for charges, e (electronic charge); for energies, kJ/mol; for B, (kJ/mol)$^{1/12}$·nm; for diffusion constant, 10^{-5} cm^2·s^{-1}; for pressure, bar. [b] New run under same conditions as models 1−4. [c] Including quantum corrections (ref 5).

Table1 description: This is a benchmark comparison of the potential energies of water simulation by Berdensen et al. for different variations of SPC water simulation model under 300K. Our data was obtained under lower temperature level (0 Kelvin), hence the lower overall stabilization of -24KJ/mol compared to -40 KJ/mol observed in this table.