From Molecular Dynamics to the Age of Machine-Learning in Aqueous Systems: A Literature Review

Final Internship Report

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Abstract

This internship provided exposure to both experimental instrumentation concepts and advanced computational approaches for studying aqueous systems. The work began with a two-week exploration of cloud chamber design, focusing on physical principles, operational challenges, and feasibility considerations for 3D-printed implementations. The remaining six weeks shifted toward a literature-based investigation of molecular dynamics (MD) simulations of water, emphasizing both historical and modern approaches. Key readings included Rahman & Stillinger's 1971 *Molecular Dynamics Study of Liquid Water* and the *Collective Burst Mechanism of Angular Jumps in Liquid Water*. These served as case studies in the evolution of MD techniques, bridging into discussions on emerging machine-learning-based potentials. The project enhanced my ability to interpret technical literature, engage in cross-disciplinary discussions, and connect classical simulation methods with modern data-driven approaches in computational chemistry.

1. Introduction

Water is one of the most studied yet still most puzzling substances in science. Its behavior at the molecular level underpins countless natural and industrial processes, from protein folding to climate regulation. Accurately modeling its structure and dynamics remains a challenge due to the interplay of hydrogen bonding, quantum effects, and collective rearrangements in its molecular network.

Molecular dynamics (MD) simulations have been a central tool in this effort since the 1970s, providing a bridge between atomic-level interactions and macroscopic properties. More recently, the development of machine-learning-based interatomic potentials has opened the door to simulations that capture subtle many-body effects with improved accuracy and efficiency.

This internship, hosted at Scientific Fabrication Lab and Condensed Matter and Statistical Physics Group at ICTP, followed a two-phase structure. In the first phase, I worked on a design study for a 3D-printed cloud chamber — an instrument for visualizing the paths of ionizing particles. Due to change in projects, in the second phase, I shifted to a literature review focused on molecular dynamics studies of liquid water and their connection to emerging ML approaches. Along the way, I participated in research discussions on supercooled water, water under electric fields, and electrolyte modeling, which provided a broader perspective on the computational chemistry of aqueous systems.

2. Background

2.1 Cloud Chambers

A cloud chamber is a particle detector that visualizes the tracks of ionizing particles as they pass through a supersaturated vapor. When a charged particle travels through the chamber, it

ionizes the surrounding gas. The vapor condenses around these ions, leaving visible trails that can be photographed or observed directly.

Designing a cloud chamber involves balancing several constraints: maintaining a supersaturated environment, controlling temperature gradients, and ensuring the chamber walls are optically clear. A 3D-printed approach introduces additional challenges, such as material compatibility with cooling methods and the need for airtight seals.

2.2 Molecular Dynamics Simulations

Molecular dynamics is a computational method in which atoms and molecules are treated as classical particles interacting via predefined force fields. The equations of motion are integrated over time, allowing researchers to simulate structural, thermodynamic, and transport properties.

For water, the key challenges include accurately modeling hydrogen bonds and accounting for the collective, cooperative nature of molecular reorientations. Early simulations, such as Rahman & Stillinger (1971), used rigid water models with effective pair potentials. While limited by computing power at the time, their results provided a foundation for decades of further refinement.

2.3 Machine Learning in Molecular Modeling

Machine learning is now being used to create interatomic potentials trained directly on quantum mechanical data. Methods such as the Smooth Overlap of Atomic Positions (SOAP) represent local atomic environments as descriptors, enabling models to learn complex potential energy surfaces from high-level calculations.

In aqueous systems, ML-based potentials promise to capture subtle features like cooperative hydrogen bond rearrangements and polarization effects without the computational cost of ab initio MD.

3. Internship Activities

Weeks 1–2: Cloud Chamber Exploration

- Researched the working principle and historical significance of cloud chambers.
- Investigated 3D printing materials and design considerations for airtight, thermally stable structures.

- Reviewed cooling methods (dry ice, heat exchangers) and vapor sources for chamber operation.
- Summarized limitations of 3D-printed designs, including potential leakage and condensation control issues.

Weeks 3–8: Literature Review on Molecular Dynamics and ML in Water

Key Tasks:

- Read and analyzed two seminal research papers in water simulation.
- Summarized computational setups, force field choices, and main findings.
- Connected classical MD results to ongoing developments in ML-driven potentials.
- Participated in weekly research discussions with group members:
    - **With Jana:** SOAP descriptors and their application to supercooled water.
    - **With Solana:** Modeling water at electric field interfaces and saline environments.
    - **With Diganto:** Approaches for electrolyte solution modeling.

4. Case Studies from Literature

4.1 Rahman & Stillinger (1971)

Simulated 216 rigid water molecules at 34.3 °C using a potential combining Lennard-Jones and Coulombic interactions. Key results included:

- Radial distribution functions showing well-defined first and second hydration shells.
- Hydrogen bond lifetimes and rotational autocorrelation functions.
- Diffusion coefficients in reasonable agreement with experiment.

4.2 Collective Burst Mechanism of Angular Jumps

This study focused on collective reorientations in liquid water, occurring in bursts rather than as isolated events. The authors linked these events to defect propagation through the hydrogen bond network and proposed that such bursts are key to understanding water's rotational dynamics on picosecond timescales.

5. Skills and Knowledge Gained

- Efficiently extracting relevant information from dense scientific literature.
- Understanding the link between molecular structure, hydrogen bonding, and bulk properties in water.
- Familiarity with SOAP descriptors and ML potential training concepts.
- Improved scientific communication through participation in expert discussions.

6. Challenges and Limitations

- No direct computational simulations due to time and resource constraints.
- Steep learning curve in transitioning from experimental instrumentation to computational theory.

7. Recommendations for Future Work

- Implement small-scale MD simulations of water using both classical and ML-based force fields.
- Compare simulation outputs directly with experimental scattering data.
- Extend literature review to confined water systems and high-pressure phases.

8. Conclusion

Although my internship began with an applied instrumentation project and shifted into a theory-driven literature review, the combination of these experiences provided a valuable cross-disciplinary perspective. I developed a foundational understanding of classical MD in aqueous systems, gained exposure to machine-learning approaches, and learned how to

navigate technical research discussions. These skills will be directly relevant in any future work involving computational modeling of complex fluids.

References

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