Scientific Background and Literature Search Summary

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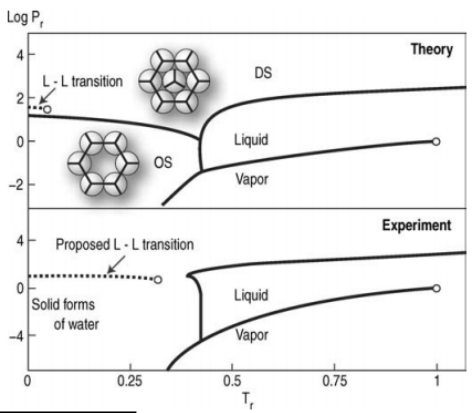
Test and Compare Current Literature of MB Water

- Run simulations with 2D and 3D MB water to compare with current research
- Compare to four state modified Muller Model used in Silverstein study [1]
- Uses 4 physical states of bulk and shell water molecules surrounding a water molecule or nonpolar solvent.
- Possible theoretical phase diagram to exhibit nteresting properties such as $_{(l)} \rightarrow_{(s)}$ transition with increasing pressure.



[1] Silverstein, K. A. T.; Haymet, A. J. D.; Dill, K. A. Molecular Model of Hydrophobic Solvation J. Chem. Phys. **1999**, 111(17), 8000-8009

For Science!

- Will provide a detailed comparison of Monte Carlo and Molecular Dynamics simulations on MB water.
- Will allow for a greater understanding of the physical properties of water.
- Will test reproducibility of several published articles.

Why Study H_2O?

- Water has many unusual features including high heat capacity (C_p), the hydrophobic effect, density anomalies (i.e. $d_{(s)} > d_{(l)}$ below 3.984^oC), isothermal compressability, etc.

- Understanding of water leads to understanding of many other natural processes (e.g. Limitations in predicting protein structures and drug interatictions and are due to our understanding of water [1])
- Importance in essentially all of science - wet chem, biologoy/biochem, environmental chem, $\cdots$

[1] Dill, K. A.; Truskett, T. M.; Vlachy, V.; Hribar-Lee, B. Modeling Water, The Hydrophobic Effect, & Ion Solvation Annu. Rev. Biophys. Biomol. Struct. **2005**, 34, 179-199

Mercedes Benz Water

- Simplified 2D model of water consisting of 2 bonds for each hydrogen and a bond combining 2 lone electron pairs.
- Interactions determined by angle, θ, by which "branches" are in relation to one another as well as Lennard-Jones Interactions.
- Resembles Mercedes Benz logo

- Used for qualitative analyses of odd properties of water
- Model is used in both Monte Carlo (MC) and Molecular Dynamics (MD) simulations.

Monte Carlo Simulations

- Statistical method based on Metropolis-Hastings Algorithm.
- Based on total energy of the system. If E_T decreases, move is accepted. If not, move may or may not be accepted depending on amount of increase of energy.
- $E_T = K_T + U_T$.
- System is allowed to equilibrate over many moves and properties of system can be extracted from that.

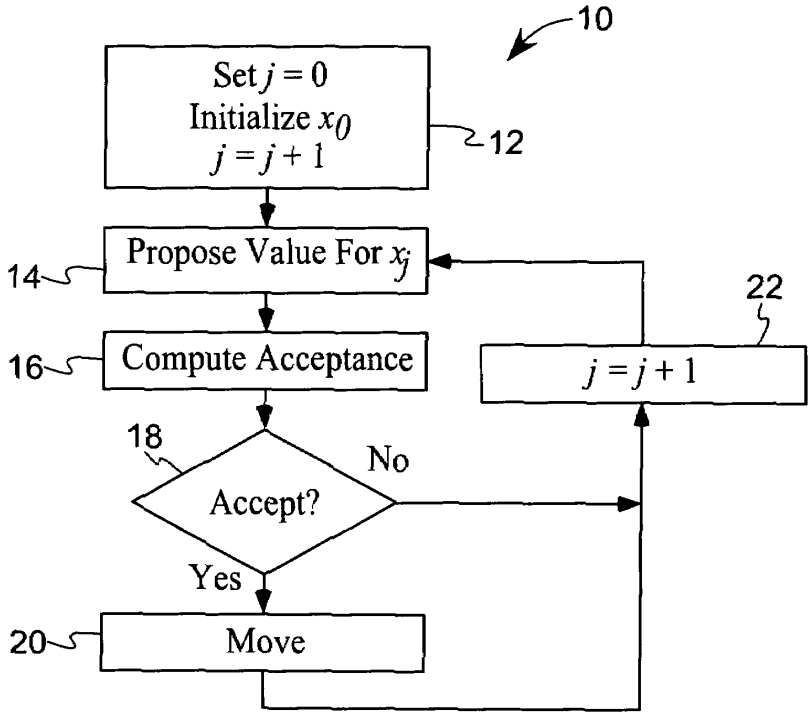
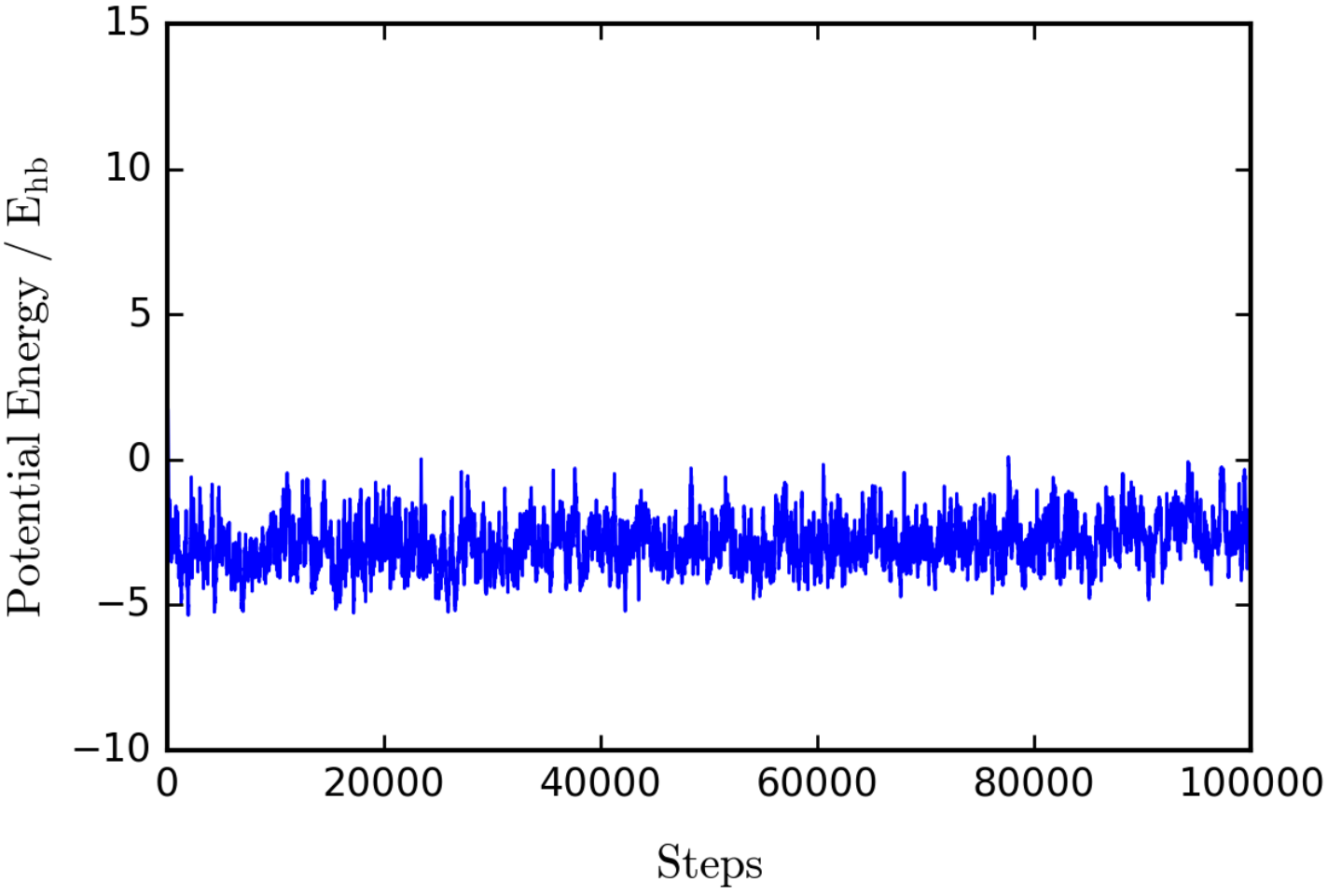
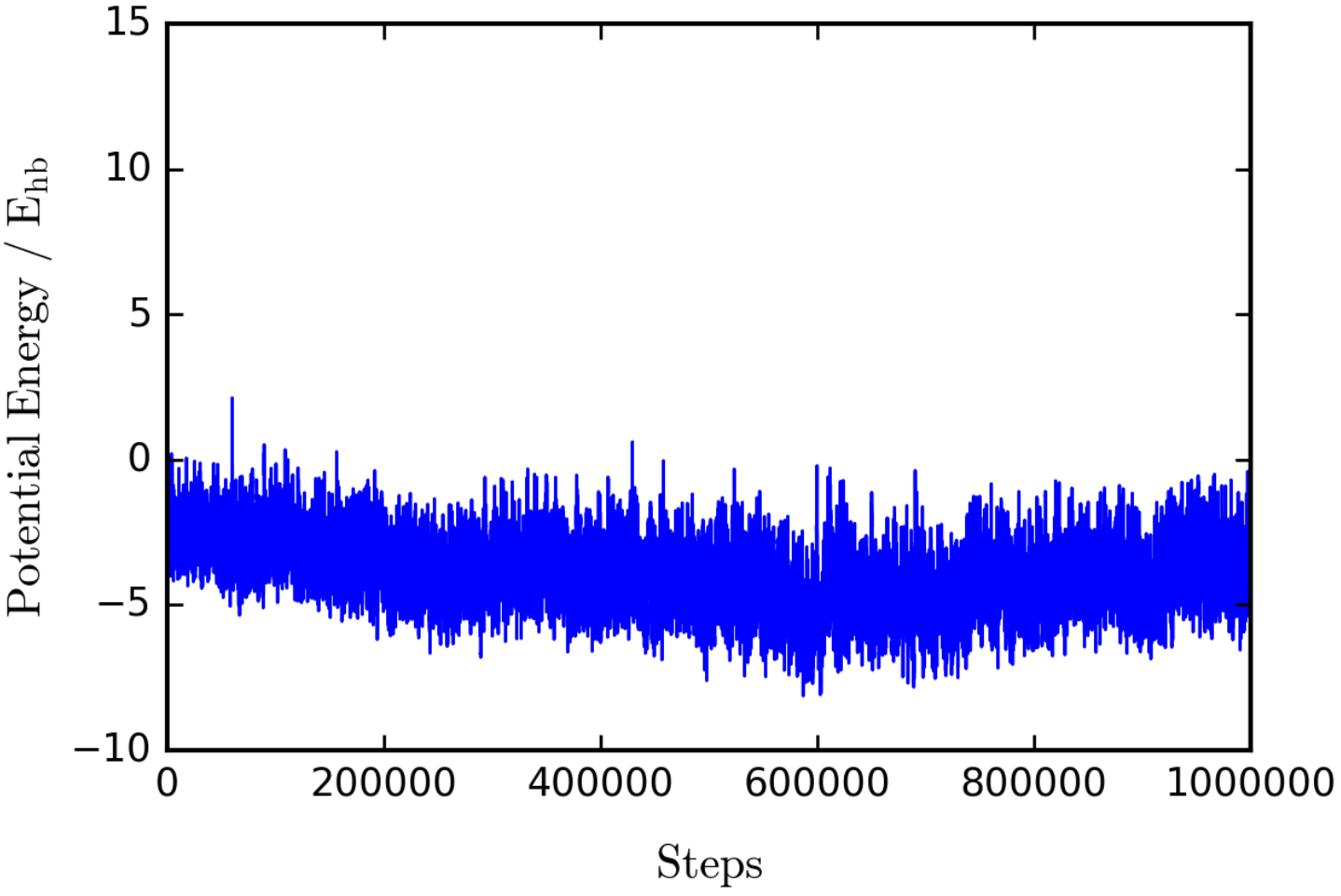


Figure 1: Diagram of the Metropolis-Hastings Algorithm

Monte Carlo Graphical Example 1



Monte Carlo Graphical Example 2



Molecular Dynamics Simulations

- A given molecule is selected, all forces acting on it are calculated, then the next position it would be located in is determined. This process is repeated. (Applied to all atoms in a system)
- Becomes very complicated very quickly including many complex partial derivatives and multiple integrals.
- Monte Carlo simulations tend to be preferred for this reason.

Does the Model Fit Reality?

- Goal is not to make a realistic model, but rather, to simulate properties of water that we want to study.
- Simulations have shown MB water to display the density anomaly, minimum isothermal compressibility, large heat capacity, and solvation trends for both ionic and non-polar compounds. [1]
- Good for qualitative properties, but does not hold as well for quantitative results

[1] Urbica, T.; Vlacy, V.; Kalyuzhnyi, Y. V.; Dill, K. A. An Imporoved Thermodynamic Peterbation Theory for Mercedes-Benz Water J. Chem. Phy. **2007**, 127, 1-4

Scientific Applications

- Test reproducibility of published articles.
- Provide teaching resources.
- Produce comparisons of MD and MC simulations in ability to simulate H_2O computationally.

Acknowledgements

- Dr. Madura
- Riley Workman
- Matthew Srnec
- Kendy Pellegrene
- Shiv[1]

[1] Sorry, Shiv, I couldn't find a folder with your last name on it.

References

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- Urbica, T.; Vlacy, V.; Kalyuzhnyi, Y. V.; Dill, K. A. An Imporoved Thermodynamic Peterbation Theory for Mercedes-Benz Water J. Chem. Phy. **2007**, 127, 1-4
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Questions?

- Study MB water to understand peculiar properties it possesses.
- Running various simulations to test MB water and Monte Carlo/Molecular Dynamics simulation methods.
- Testing results from previously published journals.
- Research can be used as a teaching resource and source of information for scientific community.