

Abstract Submitted  
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**Molecular Dynamics and Monte Carlo** WILLIAM HOLMES, University of Tennessee — Molecular Dynamics (MD) and Monte Carlo simulations were constructed and compared. The basis of the MD simulation was the classical Lennard Jones potential. Due to computational constraints, simulations were limited to a thirty-eight particle hexagonal close packed shell with outlier configuration in 2-dimensions. The MD simulations were used to observe factors such as types of transitions made and the probabilities with which they were made. Two types of Monte Carlo methods were considered. The first utilized a coarse time step model. The probabilities observed in the MD simulations were used in conjunction with a random number generator in order to determine whether or not an event would occur in the given time step. The second method used the exponential distribution to give probabilistic times for an event to occur and forced the one with the minimum time to occur. Both methods were compared to the MD simulations and exhibited similar agreement but the second was significantly faster. Current work is being done to deal with the complexity of allowing for multiple outlier particles along with interactions with the stable magic shell.

William Holmes  
University of Tennessee

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