# **Research Project Progress Report**

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Title of Project: A Coarse-grained Molecular Dynamics for Crystalline Solids

**Progress to Date**

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| Main Sources:   1. Journal Article: Xiantao, Li A Coarse-grained Molecular Dynamics for Crystalline Solids, (2010).   I’ve extensively reviewed this article making sure to understand every single line of logic. In addition to this I’ve also followed the methodology of the article and reproduced the main result of the article in the 1D-case.   1. Book: Ben Leimkuhler and Charles Matthews, Molecular Dynamics with Deterministic and Stochastic Numerical Methods, Springer (2015).   This book goes through the basics of Hamiltonian Mechanics and Simulation. It gives several examples of modelling molecules. It also shows us how to solve for the position and momentum of a particle given its Hamiltonian.   1. Book: Dirk Taeger and Sonja Kuhnt, Statistical Hypothesis Testing with SAS and R, John Wiley and Sons, Incorporated (2014).   I used this book to test Li’s claim that one of the variables that he describes in his paper is normally distributed. The source gave me a quick overview of hypothesis testing.   1. Journal Article: C. Arthur Williams Jr, The Choice of the Number and Width of Classes for the Chi-Square test of Goodness of Fit (2012).   For the use of my Chi-square goodness of fit test.   1. Journal Article: H. B. Mann and A. Wald, On the Choice Of The Number Of Class Intervals In The Application Of The Chi-Square Test   Progress:  Apart from working through and understanding the sources I’ve written 20 MATLAB files which reproduce the example of the 1D-case in the first source. The files implement the methods for solving for the position and momentum of a given Hamiltonian system shown in the second source. The Hamiltonian system I’m working with in this case is 1D particle chain under the Lennard-Jones Potential.  In addition to this I’ve written a file which tests to see whether a variable which is claimed to be normal is normal or not. It uses the Chi-Squared test for goodness of fit. This is my own addition to the paper. |

**Project Plan**

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| Outline of Project:   * The next step for the project is to implement the calculations I’ve done for a 1D particle chain in the case of a 2D lattice. The 2D lattice will be placed in the Lennard Jones Potential, and following in the steps of the paper given by Xiantao I will attempt to use a local region of the lattice to estimate the dynamics for the rest of the Lattice. * After I’ve done this, I’ll be moving onto my project report which will have the following outline. * General Introduction: In the introduction, I’m going to give a general overview and motivations behind the work I’ve done. An example of a motivation is that it aims to make simulations of materials less computationally expensive. This is because the order of magnitude of the number of atoms in a material can be around which is far too many atoms for any computer to simulate in a reasonable time. * Short Overview of Algorithms: I’ll also be giving a very short overview of the numerical integration algorithms I’ve been using in the project E.g. the Verlet Method and the Trapezium rule. * Overview Source 1: I will briefly summarise the paper given by Xianto Li, Giving the main conclusions. An example of one of the conclusion Xiantao gave is that the position and momentum of the full-scale dynamics of a given system can be expressed in terms of the position and momentum of a local region of a given system.      * 1D Particle Chain under Lennard Jones Potential: Here I will give and explain my code that I’ve written for the 1D case. The code uses the Verlet method to solve for the position and momentum of a local region of a particle chain under the Lennard Jones potential, it then uses theory presented in source 1 to attain the full-scale dynamics of the system. * 2D Lattice under a potential: Here I will give and explain my code that I plan to write for the 2D case. * Analysis/Discussion: In this section, I’ll be giving my take on the Theory presented and the calculations I’ve performed. At this moment in time, I find this project very interesting because of the applications it has in material science. It’s relevant because being able to produce large scale simulations more quickly would allow us to better understand materials better. A better understanding of materials will allow us to make products more efficiently lessening our burden on the planet. * Conclusion |

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