# **Research Project Progress Report**

Full Name: Mohamed Moallim Student No: u1408206

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

**Progress to Date**

|  |
| --- |
| Please report on your progress to date (must be typed). This would normally include a list of sources you have identified, giving comments on their relevance or role in your project and stating how far you have gotten in understanding the material. You should also summarise any calculations performed, programmes written or anything else you have achieved to date.  Main Sources:   1. Journal Article: Xianto, 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.   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.  Progress:  Apart from working through and understanding the sources I’ve written 20 MATLAB files which reproduce the example from 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. |

Do not exceed one side

**Project Plan**

|  |
| --- |
| Give a brief plan for the project (must be typed). This could either be in the form of a proposed timeline, with particular goals and time frames, or it could be in the form of an outline for the written report. In either case the plan does not have to be very detailed and you will not be penalised if in practice you deviate from this plan. However, you should have begun to think about what your report will eventually contain and how you will get there.  Outline of Project:   * The next step for the project is to implement the calculations I’ve done for a 2D 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 * 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 * Overview Source 1: I will briefly summarise the paper given by Xianto Li, Giving the main conclusions * 1D Particle Chain under Lennard Jones Potential: Here I will give and explain my code that I’ve written for the 1D case * 2D Lattice under a potential: : Here I will give and explain my code that I’ve written for the 2D case * Conclusion |

Signed:…………………...…….…………………………….(you) Date:.............................

Signed:…………………...…….…………………...….(supervisor) Date:.............................