



# Apothesis

Adding HCP and DC lattice functionalities

28.03.2023

## Basic Details

Full Name - Ujjwal Shekhar

GitHub - [@ujjwal-shekhar](#)

Email - [ujjwal.shekhar@research.iiit.ac.in](mailto:ujjwal.shekhar@research.iiit.ac.in), [ujjwalshekharofficial@gmail.com](mailto:ujjwalshekharofficial@gmail.com)

First Language - English

Location - [Hyderabad, India](#)

Timezone - +5:30 G.M.T.

## Academic Background

### Educational Details

I am currently in my sophomore year at the International Institute of Information Technology - Hyderabad, India. I am pursuing a Bachelor's of Technology in Computer Science and an M.S. by Research in Computational Natural Sciences. I have taken the following relevant courses

- Computer Programming (10.00/10.00)
- Data structures and Algorithms (9.00/10.00)
- Algorithm Analysis and Design (10.00/10.00)
- Computing in Sciences with Python (9.00/10.00)
- General Structural Chemistry (10.00/10.00)

I am also a part of my university's **C**enter for **C**omputational **N**atural **S**ciences and **B**ioinformatics lab and while I am looking to research on Machine Learning for Sciences and Network Sciences for my Master's thesis.

Most of my coursework deals with C/C++ or Python, and I have extensive experience in working with these programming languages.

## Programming Interests and Background

I have completed **all** algorithm related coursework in C/C++ and regularly take part in Sports Programming contests in which I code in C++. I am also one of the moderators of the [Programming Club of IIIT-H](#) and have worked to maintain previous codebases which include modifying and hosting a Discord Bot, updating the Club's official website and setting algorithmic puzzles for hosting Sports Programming events for the Club.

I have also implemented Parallel Tempering using Python as a part of my coursework and used MERN to implement a Reddit clone.

## Science Interests and Background

I have done Computer Science and Physics, Chemistry and Mathematics during my High School with an aggregate of 97.6% in the final exams for my High School. I also secured 99.8 percentile in Physics (with a Physics, Chemistry and Math aggregate of 99.76 percentile) in the JEE-MAINS exam conducted with over 850k applicants.

I have some basic knowledge of Markov Chains and Kinetic Monte Carlo methods but I am willing to learn further and apply these concepts to implement the deliverables for this project.

## Previous Work

### Pull Requests in the Apothesis Repository

[Will be adding soon]


### Contributions to other Repositories

[Will be adding soon]

## Motivation

### What is my motivation to take part in GSoC?

GSoC presents an exciting opportunity for me to connect with some of the most talented professionals in the industry I aspire to work in. During my exploration of potential projects, I've come to appreciate that participating in open source is not just about the project itself but also about the community it brings together. Having the opportunity to



learn from and work alongside experienced mentors and add value to the community is a significant driving force for me.

Open source projects have the potential to make a significant impact on a global scale, benefiting countless individuals in various ways. By participating in GSoC, I'll be able to be a part of a global community, contribute to impactful open source projects, and gain practical experience while learning new skills.

Overall, GSoC is an unparalleled opportunity to contribute to meaningful projects, learn from experienced professionals, and have a lasting impact on communities worldwide. These are all compelling reasons for me to participate in GSoC.

### Why do I want to work on this particular project?

I am thrilled to apply for the GSoC project idea, 'Creating new lattices for Apoptosis.' The prospect of combining my interests in solid state lattices, Markov chains, and computational sciences in this project is incredibly exciting. As a sophomore pursuing a B.Tech. in Computer Science and M.S. by Research in Computational Natural Sciences, I have developed a strong foundation in C/C++ and Python, which will enable me to make a valuable contribution to this project.

What I find particularly compelling about this project is the opportunity to work on a real-world problem using computational methods and open-source technologies. The prospect of learning about Kinetic Markov Chains and optimizing their implementation in C++ is especially intriguing to me. Moreover, this project aligns with my long-term career goals of working at the intersection of computer science and natural sciences.

By working on this project, I hope to develop my skills in software development, learn from the experiences of the mentors and the community, and contribute to the field of surface science. I am grateful for the opportunity to apply for this project and look forward to collaborating with the mentors and the community to make a meaningful impact.

### What are your expectations from us during and after successful completion of the program ?

During the program, I expect to receive guidance and support from my mentor(s) to help me navigate through the project, understand the codebase and implement the required

features. I am looking forward to receiving regular feedback on my work so that I can improve my skills and deliver high-quality work.

After successful completion of the program, I hope to have a good understanding of the project and its codebase, which will help me to continue contributing to the open-source community. I am excited to be a part of a community that is constantly evolving and has the potential to make a meaningful impact on the world. Finally, I hope to maintain a long-term relationship with the community and continue to contribute to it in the future.

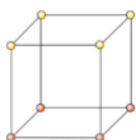
## Project Details

### What are you making?

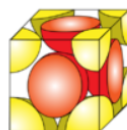
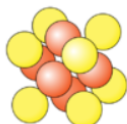
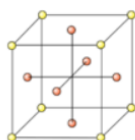
#### PROBLEM ABSTRACT

Apothesis currently uses C++ to simulate Deposition processes on solid surfaces based on KMC methods. To do this, one needs a lattice where the elementary processes can be performed. As of now, Apothesis only supports Simple Cubic and (partial) Face Centered Cubic lattice structures.

**Simple Cubic**



**Face-centered cubic**



The current lattice options available are not very extensive, they can only simulate a small subset of surface reactions. Adding HCP and Diamond lattices will turn out to be very useful.

#### WHY IS THIS USEFUL?

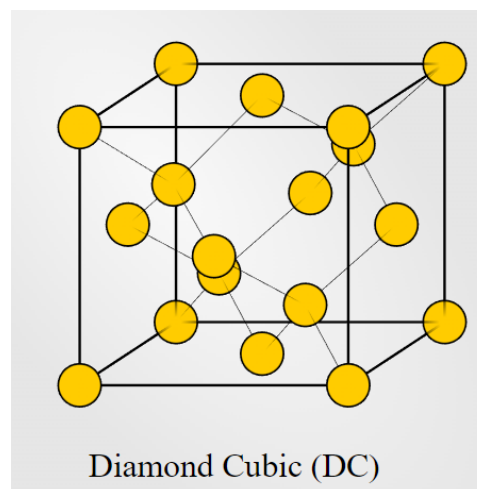
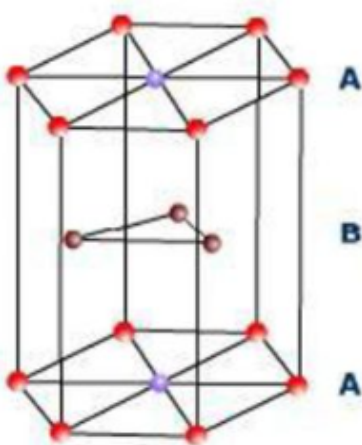
The following showcases how Graph Theory can be used to model a Simple Cubic lattice without having to bank on an assumption like "A participating species can only occupy one site at a time".

This shows how Lattice Kinetic Monte Carlo simulation can be used to study the atomic diffusion and structural

transition of Gold by modeling the problem on an HCP lattice. In aerospace, HCP materials are used for the construction of turbine blades and other high-stress components that require high strength and excellent corrosion resistance. Thus, to be able to simulate deposition of thin films over such surfaces is highly important as it might provide valuable insights and a much smaller computational cost.


Developing Interests in Chemical Vapor Deposition on diamond films shown [here](#) and [here](#) prove that adding HCP and Diamond lattice functionality will improve the user base for Apothesis and help other people simulate and gain insights for their work.

I am proposing to work on an open-source project called Apothesis. My project involves adding functionality to Apothesis for simulating hexagonal close-packed (HCP) and diamond lattices. (HCP and DC lattices shown below)



The importance of this project can be seen in the applications of lattice simulations in various fields. For example, the use of Graph Theory to model a Simple Cubic lattice without having to assume that a participating species can only occupy one site at a time is highlighted in a [scholarly article](#). Additionally, a [research paper](#) demonstrates the use of Lattice Kinetic Monte Carlo simulation to study the atomic diffusion and structural transition of Gold by modeling the problem on an HCP lattice. HCP materials are commonly used in the aerospace industry for the construction of turbine blades and other high-stress components that require high strength and excellent corrosion resistance. Therefore, simulating deposition of thin films over such surfaces is crucial as it may provide valuable insights and a much smaller computational cost.

Furthermore, the addition of HCP and diamond lattice functionality to Apothesis can improve its user base and enable researchers in various fields to simulate and gain insights for their work. The interest in [chemical vapor deposition on diamond films](#) further emphasizes the need for such functionality.



In summary, my project aims to enhance the functionality of Apotheosis by adding simulation capabilities for deposition of thin films on HCP and diamond lattices. This would help researchers in various fields to gain insights and improve their work.

## What technologies will you be using?

### C++

The codebase is mostly using C++ to implement Kinetic Monte Carlo Simulation that simulates Deposition processes.

### Python (Optional)

The codebase (as of 27th March 2023) doesn't use Python. It can be used to make scripts that carry out sample studies and generate results/plots to verify the working of the codebase.

### Make

It offers Quality of life compile options to help run multiple compile and/or run multiple files/commands by typing a single command.

## Specifications

### Availability

I am willing to spend **40 hours per week** or more after 8th May 2023. End semester examinations and paper reviews at my university conclude on May 8th, following which I have summer holidays and am unlikely to have any other obligations from GSoC should I get this opportunity.

### Communication

I don't have any personal choices related to communication platforms. I have accounts on most platforms and wouldn't mind making a new one if required.

## Milestones

### Phase I

For the first phase of the evaluations I plan to have completed the following tasks:

- Properly document the “examples” folder, in which I have made a PR showcasing a Parametric Study (along with a script to automatically run Apothesis, clean the Outputs and Plot results). [This is already ongoing]
- Read up on how to implement the HCP lattice using KMC and look for basic optimizations to improve the runtime/ space required for the same.
- Code up the implementation for the HCP lattice and procure examples to showcase it and validate it via rigorous testing. [Might spill over to the second phase]

## Phase II

For the second phase of the evaluations I plan to have completed the following tasks:

- Test and validate the HCP lattice implementation [In case any work is remaining from Phase I]
- Read up on how Diamond Lattice can be implemented using KMC and look for basic optimizations to improve the runtime/ space required for the same.
- Code up the implementation for the Diamond Lattice and procure examples to showcase and validate it via rigorous testing.
- Add proper documentation and standardize the input file format for both lattices.
- Test and ensure that there are no edge cases and/or pitfalls that might hamper the quality of the work.

## Timeline

### Week 1 [May 29th - June 5th]

- Make a clear plan of action, read up on resources on how to effectively implement KMC and familiarize with the existing SimpleCube and FCC implementations on the repository.
- Communicate with the mentors to understand the current state of the code in terms of its complexity and look at pitfalls that I should avoid before beginning to code up the HCP lattice part.
- Make and share a to-do list with the mentors with concise notes on the status of each task.

### Week 2 [June 6th - June 12th]

- Make a file format for the input file and add a document on how to use it. [OPTIONAL : Make a script/ CLI menu to help pick parameters in a much more user-friendly manner].

- Make a basic template for the HCP files and implement the basic workflow of the cpp files.
- Add proper comments and plan on exactly what to implement and confirm with the mentor on resources before starting to code.

### Week 3 [June 13th - June 19th]

- Start off with the coding process whilst also looking at good coding practices for implementing an HCP lattice file.
- Complete at least 80% of the HCP.h file so that HCP.cpp can be coded in the following week.
- Test and review if there are edge cases in the codebase.
- Document changes and detail the already added comments to the header file to make it easier for future contributors to work on.

### Week 4 [June 20th - June 26th]

- Finish off if anything left over in the HCP.h file from previous weeks.
- Start working on the HCP.cpp file while documenting all changes.
- Confirm plans with the mentors and properly read up on the Markov Chain implementation of the same.
- Code up a basic version of the lattice and test with a sample input.
- Take reviews from the mentors on the code and refactor accordingly.

### Week 5 [June 27th - July 3rd]

- Depending on the reviews further validate the code and ensure quality.
- Document the changes made and add instructions on how to use the HCP file to simulate a deposition process.
- [OPTIONAL] Add a sample study in the "examples" folder to demonstrate the HCP lattice implementation and its uses.
- Receive feedback from mentors on the implementation and work done so far.

### Week 6 [July 4th - July 10th]

- Read up on how to implement Diamond lattice using the KMC, and take note of any insights after having implemented the HCP lattice.
- Make an input file format for the Diamond lattice and document details on how to use it [OPTIONAL : Make a script/ CLI menu to help pick parameters in a much more user-friendly manner].
- Add template for the Diamond lattice file and showcase the basic workflow of the files.



- Add proper comments and plan on exactly what to implement and confirm with the mentor on resources before starting to code.

## Week 7 [July 11th - July 17th]

Same steps as [Week 3](#), but in the context of Diamond Lattice

- Start off with the coding process whilst also looking at good coding practices for implementing an Diamond lattice file.
- Complete at least 80% of the DC.h file so that DC.cpp can be coded in the following week.
- Test and review if there are edge cases in the codebase.
- Document changes and detail the already added comments to the header file to make it easier for future contributors to work on.

## Week 8 [July 18th - July 24th]

Same steps as [Week 4](#), but in the context of Diamond Lattice

- Finish off if anything left over in the DC.h file from previous weeks.
- Start working on the DC.cpp file while documenting all changes.
- Confirm plans with the mentors and properly read up on the Markov Chain implementation of the same.
- Code up a basic version of the lattice and test with a sample input.
- Take reviews from the mentors on the code and refactor accordingly.

## Week 9 [July 25th - July 31st]

Same steps as [Week 5](#), but in the context of Diamond Lattice

- Depending on the reviews further validate the code and ensure quality.
- Document the changes made and add instructions on how to use the Diamond file to simulate a deposition process.
- **[OPTIONAL]** Add a sample study in the "examples" folder to demonstrate the Diamond lattice implementation and its uses.
- Receive feedback from mentors on the implementation and work done so far.

## Week 10 [August 1st - August 7th]

- Properly comment and document any remaining parts of the code that need to be properly documented.
- Take reviews from mentors and improve the implementation if needed.
- Implement any of the "Optional" features that are remaining if time permits.

## August 8th - August 21st

- Finish any remaining tasks and get rid of backlogs and explore the next steps.
- Discuss optimizing the current implementation to improve runtimes with the mentors.
- Validate the current implementation by putting it through rigorous testing.
- Add samples to demonstrate the use cases if needed.

## Post GSoC

I would like to continue contributing to Apothesis by improving the current optimization.

- For this I plan to look at auto-vectorization and SIMD/SIMT optimizations to improve run-times.
- I also plan to explore heuristic possibilities to improve the KMC implementation and achieve much better runtimes.
- I would like to add a CLI menu for a much more user-friendly experience.