Apothesis

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Basic Details

Full Name - Ujjwal Shekhar

GitHub - @ujjwal-shekhar

Email - ujjwal.shekhar@research.iiit.ac.in, ujjwalshekharofficial@gmail.com

First Language - English

IRC nickname - [UNCLEAR]

Location - Hyderabad, India

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

Academic background -

Previous Work

[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 did you choose GFOSS?

[Will be adding soon.]

Why do I want to work on this particular project?

I am thrilled to apply for the GSoC project idea, 'Creating new lattices for Apothesis.' 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.

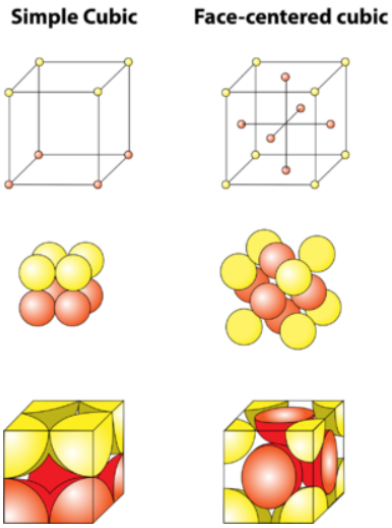
After successful completion of the program, I hope to have a good understanding of the project and its codebase, which will help me to continue contributing to the open-source community. I am excited to be a part of a community that is constantly evolving and has the potential to make a meaningful impact 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.



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 userbase 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.

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 Apotheosis 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.

How will it impact Open Technologies Alliance(GFOSS)?

[Will be adding soon]

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.

[Will be adding soon]

Milestones

Phase I

Phase II

Timeline