Creating a factory pattern

for handling lattices in Apothesis

# **Project description**

Apothesis is a generalized software for designing, simulating and analyzing deposition processes. It is based on the kinetic Monte Carlo method and consists of two main components; a lattice (e.g. simple cubic, HPC etc) and the processes (adsorption, desorption, diffusion and surface reactions) performed in this lattice. For incorporating processes inside Apothesis a factory pattern design has been developed which makes the software easy to expand. However, the lattices are developed in a rather hard coded way and it is not easy to be expanded or to add new lattices in easy way. For that, this project’s main goal is the development of a factory pattern to incorporate lattices in Apothesis through a factory pattern.

# **Personal Details**

I am an undergraduate student at Informatics and Computer Engineering. The main focus of my studies is to encompasses the ways, means and methods of human activity, aimed at creating and using of computers, computer systems and networks, automated information processing and control systems, software and automated design systems.

While the objective of the program is to train highly qualified specialists in the field of Hardware and Software Engineering, we are learning basic programming languages such as C and C++. Also, we are analyzing and creating simple algorithms so we can accomplish the given programming tasks.

Throughout my high school years at a vocational high school in the major of Applications Technician, I gained knowledge in Python programming, databases and data structures

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# **Motivation**

What is your motivation to take part in Google Summer of code?

As a student, who is not professional at programming, I want to obtain as much experience as I can, so I can become a high efficient programmer in the future. I highly believe in the importance of open-source software as open-source tools have been very important at my studies in university . I strongly believe in the development of open-source tools and I would be really excited to work on a big project such as the ones offered by the GSOC.

Why did you choose Open Technologies Alliance – GFOSS?

GFOSS is one of the largest organizations for open-source software in Greece and hosts projects from various fields, including scientific based projects. Thus, I have been looking at the software projects offered by GFOSS because of their diverse nature and my interest in projects used for scientific research.

Why do you want to work on this particular project?

Although this project differs from my field of studies, it aligns with my technical background and my will to learn how to merge my programming skills with different scientific fields. Furthermore, I may be not a professional programmer as I said previously, but I have the skills to finish the project successfully. Last but not least, I am excited to contribute to a software project with scientific impact that could be widely used by the scientific and engineering community.

# **Implementation**

As already started in the problem description, Apothesis supports lattices that are hard copied inside its structure. However, for the software to be robust and easy to expand, the lattices should be incorporated in an easy-to-use way. For that, we are going to implement a factory pattern for adding new lattices based on the factory pattern that is already implemented in Apothesis for adding processes. The entire code development will be based on an example of a 2D lattice of graphene which will be used as a test case.

Firstly, the lattice basis class will be altered and be re-designed for the lattices to be created based on a unit cell. The unit cell holds the primary positions of the particles, repeating the unit cell in space will create the lattice. The sites where the processes of Apothesis will be performed will be created after the lattice is constructed. Thus, the lattice class must hold at least:

1. The unit cell from which the lattice will be constructed
2. A vector of the sites upon which the processes will be performed. Note that the lattice particle positions may not be the same as the sites.

This lattice class will be basis which will be used in the factory pattern that we are going to develop.

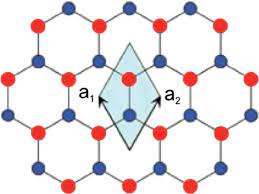


Figure 1. The graphene lattice showing the unit cell with its two primary vectors.

# **Timeline**

**May 1 - 26**

* **Community Bonding Period | GSoC contributors get to know mentors, read documentation, get up to speed to begin working on their projects**

I already have a primary communication with my mentors but during this period we will build strong communication channels for making this project a successful one.

I will build and run some cases of Apothesis and understand its structure.

I will review the literature for the theoretical/physicochemical knowledge needed for this project and based on that, along with my mentors, I will make the design of the code to be developed.

**May 27 – July 12**

* **Coding officially begins!**

Create and update the classes for building the graphene structure namely:

1. The unit cell class
2. The sites class
3. The lattice class

**July 12**

**Midterm evaluation to be submitted.**

**July 12 - August 19**

* **Work Period | GSoC contributors work on their project with guidance from Mentors**

Build the factory pattern based on the classes developed in the previous periods. Here the factory pattern already implemented in Apothesis will be used as basis.

**August 19 - 26**

* **Final week: GSoC contributors submit their final work product and their final mentor evaluation (standard coding period)**

Rap up all the source code. Build a version of Apothesis out of it. If successful used it as an example to transfer all other lattices already implemented in Apothesis under the factory pattern. Use this week in case of some work getting delayed, in case of any emergency or otherwise.

**August 26 - September 2 - 18:00 UTC**

* **Mentors submit final GSoC contributor evaluations (standard coding period)**

# **Post GSOC**

I would be more than happy to continue working on Apothesis after the completion of the project in case there are any open issues if it aligns with my university schedule.

# **Communication**

Because my schedule is oddly structured I can work on Mondays 09:00-13:00 and every other Friday 09:00-13:00. I can also work full time on weekends. I can also make adjustments on my current work schedule depending on the project’s demands