Bachelor Thesis Topic

From Scripts to Computational Materials Science Data Analysis Workflows

Motivation and Background
Multi-choice data analysis workflows are used in computational materials science (CMS) to explore and analyze materials properties. Such workflows are composed of computer programs, called codes, that implement a range of theoretical methods for characterizing chemical and physical properties of various kinds of materials; scripts that pre-process input data to the codes (e.g., to configure and parameterize the used code), and scripts that post-process the output data of the codes (e.g., to extract, visualize, and analyze the results). In this context, scientists are confronted with a huge variability of such workflows since they can choose among more than 40 codes, each further requiring different scripts to pre- and post-process data in code-specific formats.

Goals
The goal of this project is to implement a tool that integrates given scripts into ASE/Pymatgen workflows.

Description of the Task
- Getting familiar with the automated techniques get from scripts to workflows
- Implement tool to integrate these scripts into ASE/Pymatgen workflows

Research Type
Theoretical Aspects:
Industrial Relevance:
Implementation

Prerequisite
The student should be enrolled in the bachelor of computer science program, and has completed the required course modules to start a bachelor's thesis.

Skills required
Programming skills in Java or C++, understanding of, or willingness to learn, the software engineering and software analysis foundations needed for the project.

References

Contacts
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Application
Please contact me during my office hours or send me an email with the title: “[ThesisProject]-MetamorphicTestingInCMSDAWs” to se-career@informatik.hu-berlin.de