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 bachelors 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

[1] [VDS+19] Vogel T., Druskat S., Scheidgen M., Draxl C., and Grunske L.(2019). “Challenges for Verifying and Validating Scientific Software in Computational Materials Science”, se4science, Software Engineering for Science, IEEE, pp. 25-32

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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