# Bachelor/Master Thesis Topic
# Metamorphic Testing in Computational Materials Science Data Analysis Workflows

## Motivation and Background

Software testing is a crucial part of software development. It enables assurance, of correctness, completeness, and reliability of software systems. Current state-of-the-art software testing techniques employ techniques like metamorphic testing [1], which is specifically designed to test software without an oracle. The idea is to identify and refine a set of metamorphic relations between the software inputs and outputs. Just to give an abstract example, for a square root function sqrt(x) the relation x=sqrt(x)*sqrt(x) should hold under reasonable floating point accuracies. Identifying such relations is highly domain dependant and in the field of Computational Materials Science (CMS) in particular, it is still an open research question [2].

## Goals

The goal of this project is to identify, understand, and explain metamorphic relations in the field of CMS.

## Description of the Task

- Getting familiar with the automated techniques to identify metamorphic relations
- Implement tool to identify such relations in CMS DAWs
- Perform an experimental evaluation of these hidden metamorphic relation

## Research Type

| | |
|---|---|
| Theoretical Aspects: | ★★★★☆ |
| Industrial Relevance: | ★★★☆☆ |
| Implementation | ★★★★★ |

## Prerequisite

The student should be enrolled in the bachelor/master of computer science program, and has completed the required course modules to start a bachelor/master 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]     Chen T. Y., Cheung S. C., and Yiu S. M., "Metamorphic testing: a new approach for generating next test cases," HKUST-CS98-01, Department of Computer Science, Hong Kong, Tech. Rep., 1998

[2]     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

## Contacts

Lars Grunske, Humboldt-Universität zu Berlin, Institut für Informatik, Lehrstuhl Software Engineering, Unter den Linden 6, 10099 Berlin, Germany

## 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