

Project Description

The purpose of this project is to practice the various steps and tasks related to taking an existing application software and refactor it into a modular, documented project, which is easier to maintain and extend. Subtasks of the project are: setting up and using source code management and project management, adding documentation, writing a python frontend to replace the ad hoc input system, implementing additional modules that are variants of the existing modules, and adding unit and regression testing. As application software you will use the LJMD minimal MD code version that was presented during the workshop. You have to select to build either a C/C++ or Fortran based version.

Project Management

The group manager will set up a project on github.com where all sources will be maintained. All group members need to set up an account at github.com and join the project. The group will have to organize itself and distribute and schedule sub tasks.

Tasks

1. Refactor existing code: take the single file source code and break it down into separate files, each representing a module that contains a subtask of the overall simulation task.
2. Replace the ad hoc input data parsing with a python interface, so it can support reading very different file formats and can write python scripts that will set up calculations.
3. Embed documentation for users and developers into the various source files and add support to automatically extract this and translate it into a PDF file.
4. Build a library of unit and regression tests for validating individual modules and the entire application, respectively.
5. Extend the simulation infrastructure, so it can handle multiple types of atoms with different sets of parameters between different pairs of atom types.
6. Extend the simulation framework to handle new a new type of potential (Morse), a new type of run (minimization with steepest descend), and output to a different file format.