COMP3000 Minutes – First Meeting

**Details**

Attendees: Sophie Turner and Dr. David Walker.

Time: 15:15.

Location: Zoom.

**Discussion**

* David has read Sophie’s project proposal.
* David will be Sophie’s COMP3000 project supervisor.
* The project will be to create a chemistry application which uses an evolutionary algorithm (EA) to predict molecular structure.
* The project will primarily be written in Python.
* Sophie is having problems setting up the Atomic Simulation Environment (ASE) calculators in Python. David offered to help with this next week.
* David suggested using an interactive EA.
* The possibility of using inline C within Python was discussed.
* David recommended using pre-existing libraries/modules for the chemistry calculations and focussing firstly on the computer science aspects of the project.
* For visualisation, David recommended displaying a 3-dimensional model of the molecule to the user.

**Tasks**

* Sophie - Start the literature review. Try to find out what kinds of EA chemists are already using.
* Sophie - Think about the user requirements of the application. What should the interface do?
* Sophie – Look into interactive EAs.
* David – Help Sophie to set up the ASE calculators in Python.

**Next meeting details**

Date: 16/10/2020.

Time: 16:00.

Location: Teams.