COMP3000

Computing Project

2020/2021

Project Title

Molecular Geometry Optimisation Using Machine Learning

Links

Source code: https://github.com/Squidgeypea/SophieCOMP3000

Backlog : https://tasks.office.com/live.plymouth.ac.uk/en-GB/Home/Planner/#/plantaskboard?groupId=94cc8cbf-c90e-473e-a3f2-7d7d5dee52d9&planId=VmtMkciqc0GG6F--BwFrqpYAESf1

Project Vision

This program is for chemists and physicists who want to estimate and view the structures of molecules without spending hours doing calculations or using a supercomputer. Geopt is a program which uses machine learning to predict the shapes of theoretical molecules.

Risk Plan

Ref	Risk event	Likelihood 1=low 3=high	Impact 1=low 3=high	Exposure 1=min 9=max	Plan
R1	Calculations too computationally expensive	2	2	4	Use Python packages for calculations. Choose appropriate methods. Simplify calculations. Try multithreading/GPU options etc.
R2	Evolutionary algorithms take too long	3	2	6	Use fewer iterations. Use different technique, selection criteria etc. Make code simpler.

R3	Programming difficulties/lack of knowledge	3	2	6	Have regular meetings with David. Do lots of research and practice.
R4	Too much to do/not finish on time	3	3	9	Keep working throughout the year. Adjust plans if necessary. Focus on most important things first. Use Agile.
R5	Unable to get desired results from algorithms	2	1	2	Alter mutations etc. Analyse and test algorithms. Do plenty of research.

Keywords

Molecular, chemical, atoms, molecules, geometry, energy, optimisation, minimisation, Python, simulation, evolutionary, machine learning.