

Molecular Geometry Optimisation

Using Evolutionary Computation

Dissertation Project

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# Abstract

# Introduction

## Background

## Aims

The aim of this project was to create an interactive evolutionary algorithm (EA) to predict the geometric structure of a molecule or system of atoms, based only on an estimate of the system’s total potential energy.

# Literature Review

# Project Plan

## Roadmap & Sprints

Tables x to x show the roadmap, which outlined the plan for the sprints. The plan was that each sprint would be based around a user story, apart from the sprints that were reserved for the planning and testing stages of the project. Sprint zero, shown in table x, was dedicated to planning the project. Sprint one, shown in table x, was to fulfil the user story: a user wishes to create a molecule. Sprint two, shown in table x, was to fulfil the user story: a user wishes to predict a shape. Sprint three, shown in table x, was to fulfil the user story: a user wishes to use a different EA. Sprint four, shown in table x, was to fulfil the user story: a user wishes to view a molecule and its analytical information, including a potential energy surface. Sprint five, shown in table x, was dedicated to usability testing and making changes to the program. Sprint six, shown in table x, was to fulfil the user story: a user wishes to interact with the algorithm. Sprint seven shown in table x, was dedicated to usability testing and making changes to the program. Sprint eight, shown in table x, was dedicated to making finishing touches and bring the programming part of the project to an end. Sprint nine, shown in table x, was reserved for creating showcase materials and making the transition from the coding stage to the report writing stage.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | Week 1 | 09-Oct | Week 2 | 16-Oct | Week 3 | 23-Oct | Week 4 | 30-Oct |
| **Milestones** | |  | **Sprint** | **zero** |  |  | **Sprint** | **one** |  |
|  |  |  |  |  |  |  |  |  |  |
|  |  |  | **Planning** |  |  | **User story: I wish to create a molecule** | | | |
| **Plan** |  |  | **Setup** |  |  |  |  |  |  |
|  |  |  | **Literature review** | |  |  |  |  |  |
| **Test** |  |  | **Target user questionnaires** | | |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  | **Allow user to select elements** | | |
| **Application** | |  |  |  |  |  | **Create a logo** | |  |
|  |  |  |  |  |  |  | **Create UI** |  |  |
|  |  |  |  |  |  |  | **XML** |  |  |
|  |  |  |  |  |  |  | **Display the molecular formula** | | |

*Table x – Sprints zero and one.*

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | Week 5 | 06-Nov | Week 6 | 13-Nov | Week 7 | 20-Nov | Week 8 | 27-Nov |
| **Milestones** | |  | **Sprint** | **two** |  |  | **Sprint** | **three** |  |
|  |  |  |  |  |  |  |  |  |  |
|  |  | **User story: I wish to predict a shape** | | |  | **User story: I wish to use a different EA.** | | | |
| **Plan** |  |  | **Update risk assessment for COVID** | | | **Try an EA which alters one atom at a time.** | | | |
|  |  | **Try an EA which makes many molecules and compares them.** | | | |  |  |  |  |
| **Test** |  | **See if the EA works to decrease energy** | | | | **Try to get a better structure prediction than before.** | | | |
|  |  | **See if the molecule's shape is displayed in the cell properly** | | | | **Test num iterations, E calcs, array changes.** | | | |
|  |  | **Make the EA** | |  |  |  | **Make the EA.** | |  |
| **Application** | | **Improve exception handling** | | |  | **Try without crossover and remove all parents.** | | | |
|  |  | **Choose EA parameters** | | |  | **Move from test area to application.** | | | |
|  |  | **Create models of the molecule** | | |  |  |  |  |  |

*Table x – Sprints two and three.*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | Week 9 | 04-Dec | Week 10 | 11-Dec |
| **Milestones** | |  | **Sprint** | **four** |  |
|  |  |  |  |  |  |
|  |  | **User story: I wish to view molecule, info & PES** | | | |
| **Plan** |  |  |  |  |  |
|  |  |  |  |  |  |
| **Test** |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  | **Potential energy surface plot** | | |  |
| **Application** | | **Display best molecules** | | |  |
|  |  | **Annotations** | |  |  |
|  |  | **Display information (angles, distances)** | | | |
|  |  | **Use of colours** | |  |  |

*Table x – Sprint four.*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | Week 11 | 18-Dec | Christmas holiday | Week 12 | 15-Jan |
| **Milestones** | | **Sprint** | **five** | Christmas holiday | **Sprint** | **five** |
|  |  |  |  | Christmas holiday |  |  |
|  |  | **Testing** |  | Christmas holiday | **Testing** |  |
| **Plan** |  | **Feedback & changes** | | Christmas holiday | **Feedback & changes** | |
|  |  | **Fixes & improvements** | | Christmas holiday | **Fixes & improvements** | |
| **Test** |  | **Usability tests** | | Christmas holiday | **Usability tests** | |
|  |  |  |  | Christmas holiday |  |  |
|  |  |  |  | Christmas holiday | **Act on user feedback** | |
| **Application** | |  |  | Christmas holiday | **Fix errors & bugs** | |
|  |  |  |  | Christmas holiday |  |  |
|  |  |  |  | Christmas holiday |  |  |
|  |  |  |  | Christmas holiday |  |  |

*Table x – Sprint five and the Christmas holiday.*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | Week 13 | 22-Jan | Week 14 | 29-Jan |
| **Milestones** | |  | **Sprint** | **six** |  |
|  |  |  |  |  |  |
|  |  | **User story: I wish to interact with the algorithm** | | | |
| **Plan** |  |  |  |  |  |
|  |  |  |  |  |  |
| **Test** |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  | **Implement plot limits in perAtom** | | |  |
| **Application** | | **Include buttons etc for interactions** | | | |
|  |  | **Make user interface for choosing settings** | | | |
|  |  | **Let user choose the algorithm** | | |  |
|  |  | **Let user set cell boundaries** | | |  |

*Table x – Sprint six.*

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | Week 15 | 05-Feb | Week 16 | 12-Feb | Week 17 | 19-Feb | Week 18 | 26-Feb |
| **Milestones** | |  | **Sprint** | **seven** |  |  | **Sprint** | **eight** |  |
|  |  |  |  |  |  |  |  | Finish code | |
|  |  |  | **Testing** |  |  |  | Final fixes & clean up | | |
| **Plan** |  |  | **Feedback & changes** | |  |  | Start writing report | |  |
|  |  |  |  |  |  |  |  |  |  |
| **Test** |  |  | **Usability tests** |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
|  |  |  | **Make changes from user feedback** | | | | **Make changes from user feedback** | | |
| **Application** | |  | **Find and fix bugs** | |  |  | **Find and fix bugs** | |  |
|  |  |  | **Tidy up** |  |  |  | **Tidy up** |  |  |
|  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |

*Table x – Sprints seven and eight.*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | Week 19 | 05-Mar | Week 20 | 12-Mar |
| **Milestones** | |  | **Sprint** | **nine** |  |
|  |  |  |  | **Submit showcase materials!** | |
|  |  |  | **Showcase materials** |  |  |
| **Plan** |  |  | **Start writing report** |  |  |
|  |  |  |  |  |  |
| **Test** |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
| **Application** | |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |

*Table x – The final sprint of the code, leading to the showcase submission.*

## Risk Assessment

## Legal, Social, Ethical and Professional Matters

# Implementation

## Design Patterns & Programming Conventions

## Technologies Used

## Energy Calculators

## User Interface

## Timeline

# Algorithms

# User Feedback

User feedback was sought in three stages, at sprints zero, five and seven. Originally, it had been planned that the second stage of user feedback would be conducted at sprint four, but it was decided that this would be more fruitful if it was moved to sprint five to allow work to be done on the user interface first, as usability testing could be difficult and confusing if it was conducted without a substantial user interface.

# Discussion & Evaluation

# Conclusions

# Suggestions

# References

Include links to my own work?

# Appendices

## Appendix A - Something