Project Plan
WebMGA 3.0: Refinement of an Interactive Viewer for Coarse-Grained Liquid Crystal Models

REDACTED

10th November 2023

Abstract

Produce, document, and benchmark an enhanced version of an existing web-based tool for visualising coarse-grained liquid crystal models. Provide insights into related computer graphics performance and optimisation.

1 Supervisor Information

- Guido Germano, Professor of Computational Science
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2 Aims and Objectives

- Fulfill any further requirements from relevant academic stakeholders.
- Identify and correct unexpected or unintuitive program behaviour.
- Address missing features and shortcomings identified by previous dissertations.
- Implement trivial usability enhancements (labels and scales etc.)
- Test using new configurations such as those using other specialised particle shapes or much larger molecule counts (attained from academic stakeholders or perhaps through generation).
- Identify performance bottlenecks and attempt to identify and apply optimisations. Analyse and compare performance resulting from enhancements.
- Comment on performance and effectiveness of optimisations (e.g. backface culling) in the particular case of configurations consisting of a very large numbers of molecules (implement new benchmark in place of unrealistic existing one).
- Investigate efficiency of different structures for storing molecular configurations (e.g. LAMMPS .cnf format vs current .json format).

3 Expected Outcomes / Deliverables

- A working, enhanced, version of WebMGA featuring no feature regressions.
- Documentation to allow further development of WebMGA.
- Reporting on optimisations to the WebMGA rendering process and their performance impact, with the intention to provide more general comments on computer graphics in other similar situations.
- Feedback from relevant academic stakeholders.
- New molecular configurations for other relevant scenarios.
- Strategies for testing and evaluating contributions.
- Sufficient documentation of any scientific background knowledge required to understand implementations.

4 Work Plan

- Summer to late September
  - Meet supervisor
  - Perform background investigation of topic (i.e. read existing reports and investigate existing WebMGA from a user perspective)
- Up to late October
  - Wait for feedback from academic stakeholders
  - Identify bugs and gaps in existing features
  - Discuss important scientific information with supervisor
  - Begin familiarising with existing WebMGA codebase, particularly JavaScript, NodeJS, React, and threejs
- Late October to early February
  - Work on aims and objectives specified
  - Submit project plan, interim report as required
- Early to mid February
  - Lock features and analysis to be undertaken for rest of project
  - Outline structure of report
  - Begin preparing video presentation
- Mid February
  - Finalise and deliver video presentation
  - Aim to complete bulk of implementation
  - Perform analysis work

- Second half of Term 2
  - Focus on final report
  - Freeze development, aim only to fix bugs identified in analysis and report production
- End of Term 2
  - Discuss report with supervisor
  - Use feedback to work on further drafts
- Start of Term 3
  - Submit final version to supervisor
  - Perform any final report tweaks
  - Submit work completed by deadline

5 Ethical Concerns

I do not forsee this project requiring ethical approval. Any libraries or data used will be included compliant with relevant licenses, or not used if this is not possible. If any molecular configurations are provided from externally, they will be credited as requested.