Interim Report
WebMGA 3.0: Refinement of an Interactive Viewer for Coarse-Grained Liquid Crystal Models

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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

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2 Progress

- Various bugfixes
  - Bounding box loading issues fixed
  - Fixed some incorrectly implemented keyboard controls
  - Fixed issues with model and renderer synchronisation
- Explored improved director calculations
  - Found to be impractical to implement due to poor performance and quality (i.e. limited functionality) of array mathematics libraries for JavaScript
- Re-implemented axes to be more useful
  - Transformed to a more appropriate screen position
  - Added director indicator
  - Colour based on director
  - Required changing render and model synchronisation to fix axes update "lag" bug
- Re-implemented colouring from director

  - Changed colouring definition from sampling a predefined palette, to a hue derived linearly from the vector dot product with the director

- Enhanced re-implementation of shape generation
  - Re-implement and simplify vertex generation for sphere, ellipsoid, spherocylinder, spheroplatelet, cut sphere
  - Cut sphere was previously erroneously cut from both ends
  - Implementation of cap shape
  - Implementation of lens shape
  - Changed model mesh complexity definition
    * Include a larger range of values
    * Move value increments to a logspace (powers of 2) due to diminishing returns of visual quality as complexity increases
    * Drastically simplified triangle generation from vertices
    * Removed mesh duplication previously present
    * Simplified normal generation
- Implementation of importing molecule configuration from standard .cnf files more commonly used in actual molecule simulation
- Prototype code for generating large configurations from tiling of smaller configurations (aiming to produce a more realistic benchmark)
- Viability investigation for distance based variable LOD
  - Found to conflict with existing InstancedMesh implementation for instanced rendering (conflicts with existing optimisation), will be revisited later

3 Work to Complete

3.1 Up to mid/late February

- Better axis labelling (i.e. arrowheads and letters)
- Fix significant model/UI value synchronisation issues
- Attempt to implement distance based variable level of detail either alongside instanced rendering if possible, or in place of it, and compare performance. Remove if found to be inefficient
- Improve benchmark to use a more realistic molecule configuration
- Further investigation of possible performance enhancements
- Fix separate director calculation issue for configurations with multiple molecule shapes (only a single director should be calculated)
- Implement improved image export functionality

  - E.g. specify output format based on common printing properties (size/dpi)

- Verify lens/cap/cut sphere coordinate definitions (i.e. where the centre is defined relative to mesh) with an academic working with these shapes
- Lock future project scope

3.2 Up to mid March

- Improve documentation of existing code
- Perform performance comparisons comparing combinations of optimisations implemented
- Verify experimentally whether CPU performance becomes the limiting for rendering speed in very large configurations
- Document all new implementations up to this point in. Address successes, failures, and compromises
- Continue (with reduced focus) any implementation which did not meet previous target deadline
- Semi-final code completion

3.3 By 22nd March

- Prepare video preview

3.4 By 12th April

- Document performance comparisons in report
- Document relevant scientific background (e.g. properties of molecule configuration such as director, use cases)
- Comment on scope for improvement, provide relevant research
- Semi-final report draft completion

3.5 By 26th April

- Address previous draft feedback
- Project completion