



WebMGA 3.0

Refinement of an Interactive Viewer for Coarse-Grained Liquid Crystal
Models

Candidate Number: GYWT8¹

MEng Computer Science

Supervisor: Guido Germano

Submission Date: 26th April 2024

¹**Disclaimer:** This report is submitted as part requirement for the MEng in Computer Science at UCL. It is substantially the result of my own work except where explicitly indicated in the text. The report may be freely copied and distributed provided the source is explicitly acknowledged.

Abstract

TODO

Contents

0.1 Acknowledgements	1
1 Introduction	2
2 Context	3
2.1 Molecular Graphics	3
2.2 Liquid Crystal Modelling	4
2.2.1 Director	4
2.2.2 Periodic Boundary Conditions	4
2.2.3 Molecule Shapes	5
3 Requirements and Analysis	6
4 Design and Implementation	7
4.1 Colour from Director	7
4.1.1 WebMGA 2.0 Implementation	7
4.1.2 WebMGA 2.0 Bugs	7
4.1.3 Improvement Goals	7
4.1.4 WebMGA 3.0 Implementation	7
4.1.5 WebMGA 3.0 Bugs	7
4.2 Axes	7
4.2.1 WebMGA 2.0 Implementation	7
4.2.2 WebMGA 2.0 Bugs	9
4.2.3 Improvement Goals	9
4.2.4 WebMGA 3.0 Implementation	10
4.2.5 WebMGA 3.0 Bugs	11
4.3 Shapes	11
4.3.1 WebMGA 2.0 Implementation	11
4.3.2 WebMGA 2.0 Bugs	12
4.3.3 Improvement Goals	12
4.3.4 WebMGA 3.0 Implementation	12
4.3.5 WebMGA 3.0 Bugs	24

4.4	File types	25
4.4.1	WebMGA 2.0 Implementation	25
4.4.2	WebMGA 2.0 Bugs	25
4.4.3	WebMGA 3.0 Implementation	25
4.4.4	WebMGA 3.0 Bugs	26
4.5	Periodic Repetition	27
4.5.1	Improvement Goals	27
4.5.2	WebMGA 3.0 Implementation	27
4.5.3	WebMGA 3.0 Bugs	28
4.6	Optimisations	28
4.6.1	WebMGA 2.0 Implementation	28
4.6.2	WebMGA 2.0 Bugs	28
4.6.3	WebMGA 3.0 Implementation	28
4.6.4	WebMGA 3.0 Bugs	28
4.7	Miscellaneous Improvements	29
5	Analysis and Testing	30
5.1	Level of Detail Performance	30
5.2	Configuration Visualisations	30
6	Conclusions and Evaluation	31
6.1	Achievements	31
6.2	Evaluation	31
6.3	Future Work	31
A	Appendices	34
A.1	Project proposal	34
A.2	Interim Report	38

0.1 Acknowledgements

This project was undertaken with the supervision of Guido Germano, University College London. It is a continuation of work by Eduardo Battistini (2021) and Yue He (2023), both University College London.

Giorgio Cinacchi, Autonomous University of Madrid, provided useful insight for certain parts of the project. For implementation of the lens molecule geometry, some sample molecule configurations and associated guidance was provided.

Chapter 1

Introduction

WebMGA 3.0 is a visualisation tool for molecular simulation outputs which refines on previous versions by Battistini [1] and He [2]. It provides a more modern, maintainable, and accessible alternative to the older QMGA tool by Gabriel, Meyer, and Germano [3]. The program is available as a web app at <https://joe-down.github.io/WebMGA-3>, with source code at <https://github.com/joe-down/WebMGA-3>. Development utilised JavaScript with the React[6] framework and three.js[7] 3D graphics library. This project aimed to fix existing issues in WebMGA and further enhance the existing feature set.

This report provides a background summary explaining the requirements and terminology for molecular simulation rendering (Chapter 2), descriptions for the changes required and made for WebMGA 3.0 (Chapters 3 and 4), and quantitative summaries for performance improvements and qualitative analysis of rendered systems (Chapter 5). Finally, achievements are summarised and the project successes evaluated (Chapter 6).

Chapter 2

Context

2.1 Molecular Graphics

The ability to visualise outputs from molecular simulations, particularly in the domain of liquid crystals, is important for understanding and communicating findings. QMGA[3] is a tool which can be used to generate 3D graphical representations of molecular configurations. Despite being unmaintained since 2009[8], it remains in active use to this day, having been used within the last year in publications by notable authors such as Ramírez González and Cinacchi [9] and Mazzilli, Satoh, and Saielli [10]. While another visualisation tool exists within the liquid crystal domain, LCview[11, 12], it produces plots of director and/or potential fields, rather than showing the structure of large multi-molecule system.

Since QMGA has not been updated in so long, it continues to depend on the severely dated Qt 3 framework (Qt 4 was released in 2005, 2 years before QMGA was released) requiring the installation of unmaintained and difficult to acquire libraries (e.g. the Debian Linux distribution removed all Qt 3 libraries in 2012[13]). Additionally, since the program is distributed as source code, it must be manually built by the user which is not trivial for inexperienced users. This is complicated further by the fact that modern C compilers fail without certain modifications to the source code (described by Battistini [1] in their “QMGA Compilation Issues Report”). All of these problems make installation on a modern system a significant barrier to usage.

WebMGA is a project begun by Battistini [1] in 2021 which aims to address this accessibility issue whilst replicating the functionality of QMGA. It was continued in 2023 by He [2]. It’s written in JavaScript using the React[6] framework with the three.js[7] library for 3D rendering. This addresses the accessibility issues of QMGA since it can be easily accessed using just a web browser. While WebMGA contains full functionality for rendering most molecule configurations from QMGA, it still has performance and functionality limitations, as well as some bugs. WebMGA 3.0 aims to address a majority

of these issues.

2.2 Liquid Crystal Modelling

Most details regarding molecular simulation is not required to understand the implementations made for this project. Some key concepts which will be used throughout are defined in the following subsections, based on Allen and Tildesley [14] except where cited otherwise.

2.2.1 Director

Under a coarse-grained potential model, liquid crystal configuration have a long-range orientational order, and sometimes also a long range positional order. An order represents a preferred alignment for molecules within that system[15]. The orientational order can be described by a magnitude S , and a direction \mathbf{n} . \mathbf{n} is typically referred to as the director. Both S and \mathbf{n} can be derived from the order tensor \mathcal{Q} , which is defined as follows for a system containing N molecules each with unit vector principal axis direction \mathbf{e} ,

$$\mathcal{Q} = \frac{3}{2N} \sum_{i=1}^N (\mathbf{e}_i \otimes \mathbf{e}_i) - \frac{1}{2} \mathbb{I} \quad (2.1)$$

$$\mathbf{e}_i = \begin{pmatrix} \mathbf{e}_{ix} \\ \mathbf{e}_{iy} \\ \mathbf{e}_{iz} \end{pmatrix}. \quad (2.2)$$

n can be defined as the direction which maximises S and is obtainable by diagonalising \mathcal{Q} and taking the eigenvector corresponding to the largest eigenvalue (which is itself S).

Since the director is a useful property for describing and understanding a system, it is convenient to be able to visualise both the director itself and how each molecule in the system aligns with it. Implementation of a director axis and director based axis colouring is discussed further in Sections 4.1 and 4.2.4, while molecule colouring based on director alignment was already implemented by Battistini [1].

2.2.2 Periodic Boundary Conditions

Typically molecular simulations can only be performed on small systems of $10 < N < 10,000$ molecules due to speed and/or storage constraints. With systems of this size, which is insufficient for simulating bulk liquids. Periodic boundary conditions allow modelling only a portion of an entire system[3], where an infinite lattice is simulated by repeating a smaller simulation box[16]. In each repeated boxes, periodic images of the molecules in the simulation box move in the exact same way. When a molecule leaves through a face

of the simulation box, one of its periodic images enters through the opposite face of the simulation box with the same movement properties.

Due to the necessary use of periodic boundary conditions for many molecular simulations, it may be useful to visualise a larger portion of the infinite lattice, as discussed in Section 4.5. Folding and unfolding of molecules based on periodic boundary conditions was already implemented by He [2].

2.2.3 Molecule Shapes

Molecular simulations model liquids as a collection of molecules. Each molecule has a shape approximately representative of the positions and sizes of the atoms they consist of. Allen [17] identifies a range of appropriate molecule geometries commonly used for hard-particle simulations; specifically the hard sphere, prolate ellipsoid, spherocylinder, double cut sphere, and spheroplatelet. In addition to these, QMGA implements the eyelens shape. Cinacchi and Torquato [18] have researched packings of molecules with a biconvex lens shape. All of these molecule shapes should be supported by WebMGA to successfully visualise models of each type. Implementations for geometry generation of all required types are discussed in Section 4.3.

Chapter 3

Requirements and Analysis

TODO

Chapter 4

Design and Implementation

4.1 Colour from Director

4.1.1 WebMGA 2.0 Implementation

4.1.2 WebMGA 2.0 Bugs

4.1.3 Improvement Goals

4.1.4 WebMGA 3.0 Implementation

4.1.5 WebMGA 3.0 Bugs

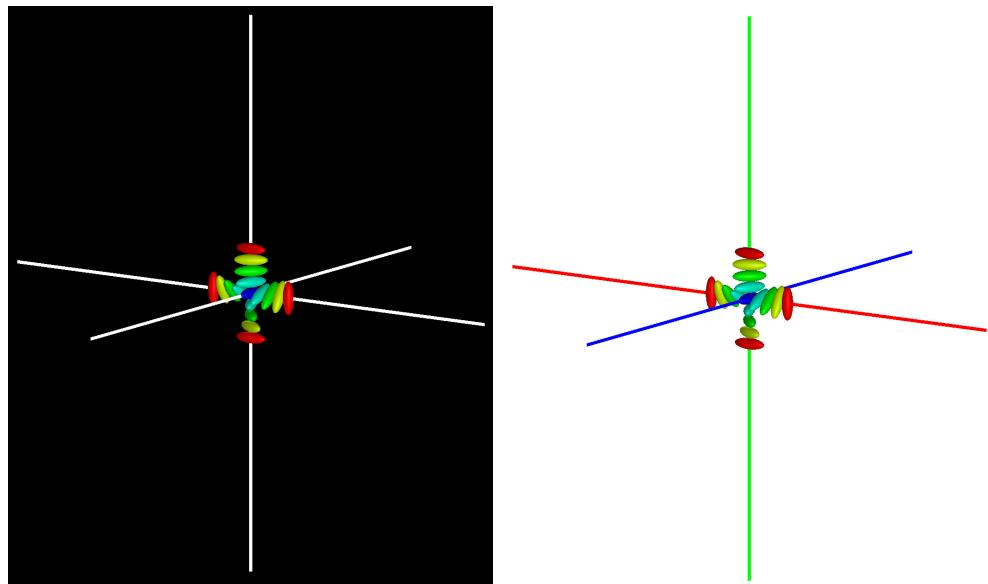
4.2 Axes

4.2.1 WebMGA 2.0 Implementation

In WebMGA 2.0, the 3D axes are displayed as shown in Figures 4.1a and 4.1b, and controlled through the user interface as shown in Figure 4.1d (visibility and colour toggles).

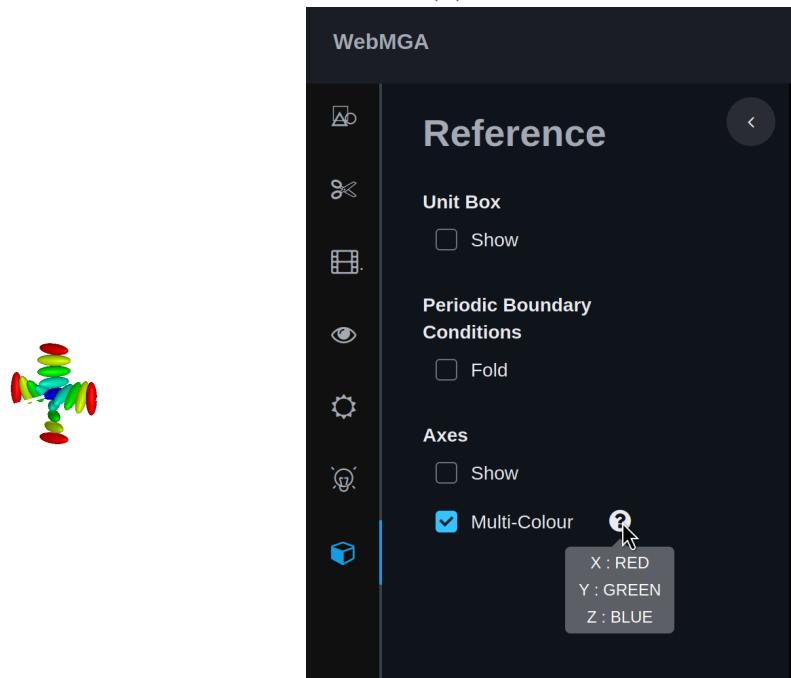
Axes take the form of three lines of fixed lengths in the x , y , and z directions. Each line’s midpoint is the lab fram coordinate $(0, 0, 0)$, where all axes meet. Axes extend in both positive and negative directions. They are not shown by default and, when first enabled, are uncoloured. When coloured, the x axis is red, the y axis is green, and the z axis is blue.

Visibility is toggled using the “Show” button and colour is toggled with the “Multi-Colour” button. A question mark icon is next to the “Multi-Colour” which shows a tooltip when hovered specifying the axis colour scheme.



(a) Colour disabled

(b) Colour enabled



(c) Colour disabled (light background)

(d) GUI controls

Figure 4.1: Axes in WebMGA 2.0

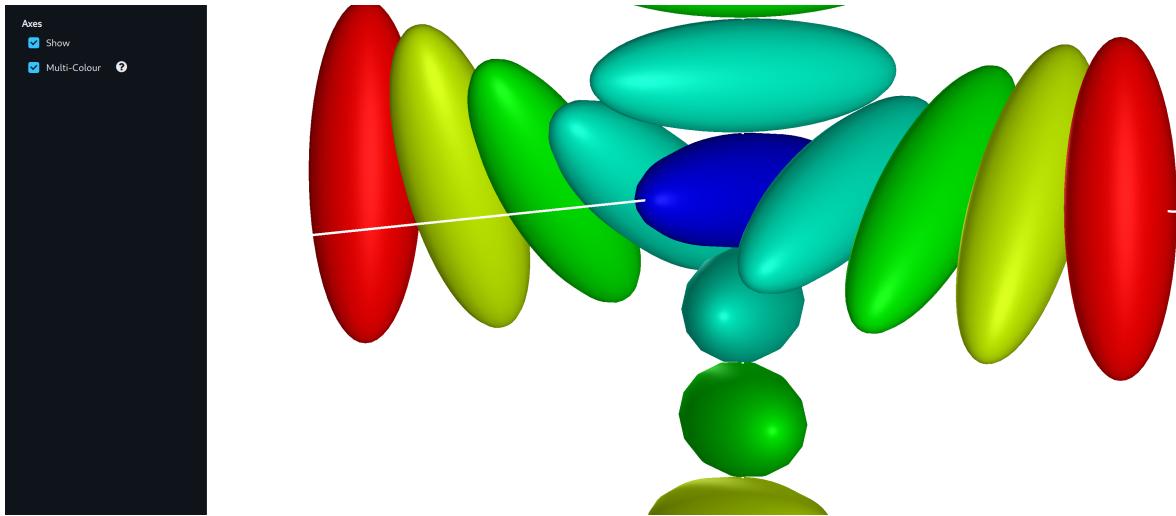


Figure 4.2: Bug where axes are not coloured despite the “Multi-Colour” toggle being enabled when axes are first enabled.

4.2.2 WebMGA 2.0 Bugs

When the axes are toggled to visible for the first time, if the “Multi-Colour” toggle has not been interacted with first, the axes will be uncoloured, despite the “Multi-Colour” toggle being enabled by default. This is shown in Figure 4.2. To enable colour for the first time, the ”Multi-Colour” toggle must be disabled and then re-enabled.

When the environment is set to light mode (white background) with coloured axes disabled, the axes become difficult to view since they retain a white colour as default, blending into the background as shown in Figure 4.1c.

4.2.3 Improvement Goals

- Axes are unlabelled
 - Axes should be changed to extend only in the positive direction
- Director(see Section 2.2.2 for definition) is not shown
 - An additional line should be shown indicating director direction
- Colours should be labelled or meaningful
 - Colour axes according to angle with director (as in TODO REFERENCE)
- Axes should not be obscured
 - Place axes in screen corner rather than centre
- Axes should be clearly distinguishable

- Ensure axes retain contrast with background under light and dark views

4.2.4 WebMGA 3.0 Implementation

Axes Positions

The existing implementation was found to be needlessly convoluted so was largely stripped out. For example, coloured and uncoloured axes were implemented entirely separately, resulting in a large amount of duplicated code and convoluted logic flow. The bug identified in WebMGA 2.0 regarding uncoloured axes showing with "Multi-Colour" enabled, for example, was found to occur due to incorrect colour object initialisation, meaning what should be "Multi-Colour" axes showed as uncoloured since the colours are not defined when these lines are loaded the very first time.

In the new axes code, they are simply defined in terms of an axes centre point, three axes vectors, and an axis length scale. The axes vectors are handled in the lab frame so are trivially defined as $x = (1, 0, 0)$, $y = (0, 1, 0)$, and $z = (0, 0, 1)$.

Since the axes centre needs to remain in a fixed position on screen at all times, it needs to be defined relative to the camera. Three.js provides a method on any world object which converts from object relative coordinates to the lab frame, so this is used to trivially place the axes centre into the lab frame as required. Since this relationship changes when an object, in this case the camera, moves, the axes centre must therefore be redefined on any camera movement. This process also does not account for changes to intrinsic camera properties, importantly camera zoom. The axes therefore need to be scaled proportionally to the camera's zoom level on any zoom change.

Using the lab frame centre point and the axes vectors and scales, axis lines are trivially defined as,

$$l_0 = c \quad (4.1)$$

$$l_1 = c + szv \quad (4.2)$$

where l_0 and l_1 are the axis line start and end, c is the axes centre, v is the axis vector, s is the axis scale factor, and z is the zoom factor of the camera. These can be recalculated and applied on every camera change. A Three.js Line object is constructed for each axis using the line start, end, and a colour.

Director

Plotting the director is made simple using the above setup. A new axis is simply defined using Equations (4.1) and (4.2), with v set to the already computed director vector (TODO show where this was done).

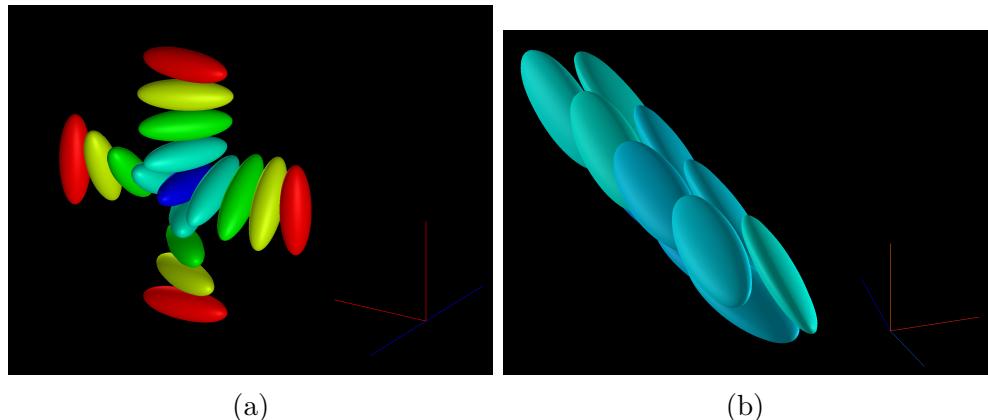


Figure 4.3: Axes in WebMGA 3.0

Axes Colouring

It was decided that a meaningful colouring for the axes lines (including the director) would be using the same colour scheme as for molecule colour (TODO show where). This can be done easily since all axes have a defined direction vector which can be passed to the TODO COLOURFROMDIRECTORNAME function (TODO show where). The resulting colour is simply passed as part of the Line object constructor.

Axes Summary

Some result can be viewed in Figure 4.3.

GUI Implementation

TODO discuss UI

4.2.5 WebMGA 3.0 Bugs

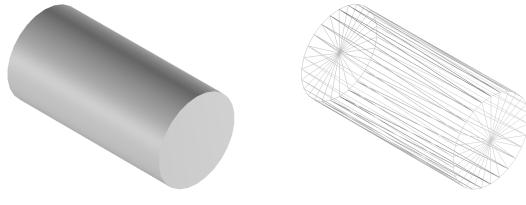
TODO

4.3 Shapes

4.3.1 WebMGA 2.0 Implementation

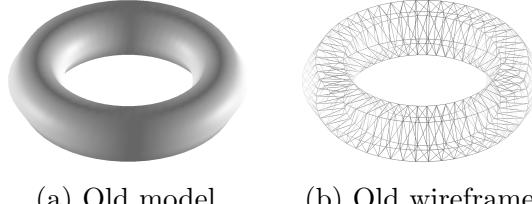
WebMGA 2.0 implements the following molecule shapes:

- Sphere (Figure 4.10)
- Ellipsoid (Figure 4.11)
- Spherocylinder (Figure 4.21)



(a) Old model (b) Old wireframe

Figure 4.4: Cylinder



(a) Old model (b) Old wireframe

Figure 4.5: Torus

- Spheroplatelet (Figure 4.12)
 - Cut Sphere (Figure 4.15, implemented as a double cut sphere)
 - Cylinder (Figure 4.4)
 - Torus (Figure 4.5)

Notably missing but useful are the single cut sphere, the spherical cap, and the lens. The cylinder and torus shapes are present since the three.js library provides easily callable predefined meshes, however serve little practical purpose since no realistic molecular configuration would model using these.

4.3.2 WebMGA 2.0 Bugs

4.3.3 Improvement Goals

- Problem
 - Fix

4.3.4 WebMGA 3.0 Implementation

Sphere

Key to the new shape implementations is the implementation for the sphere (Figure 4.10, parameter “Radius”). The sphere mesh is generated by sampling points across the sphere’s

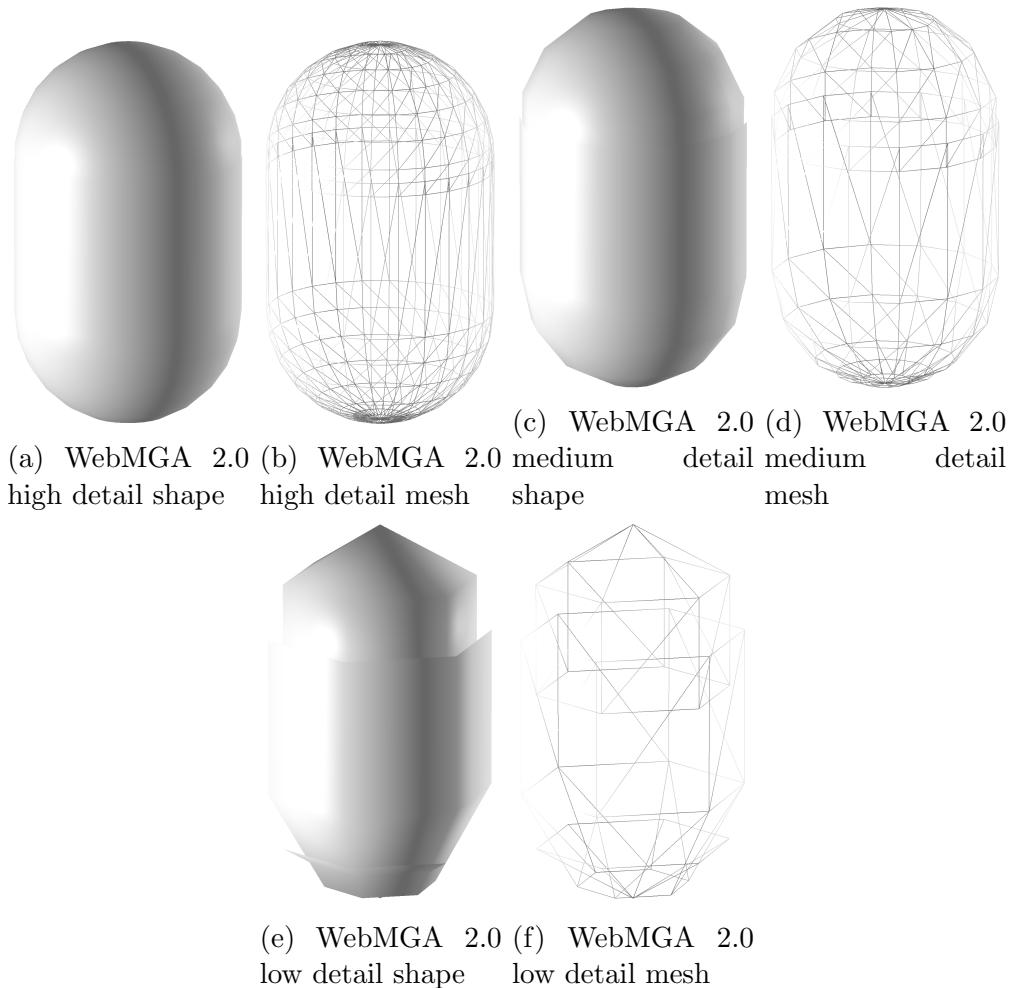


Figure 4.6: Bad spheocylinder mesh generated by WebMGA 2.0

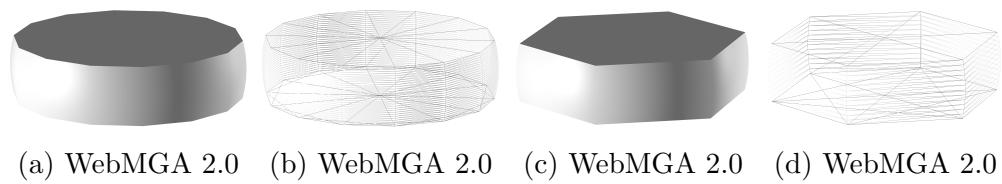
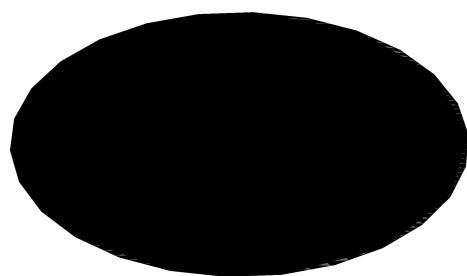
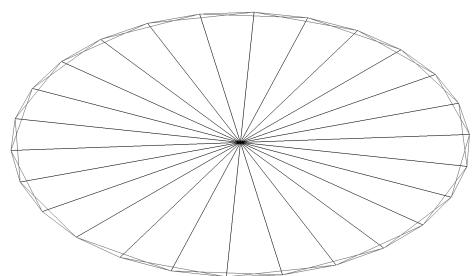


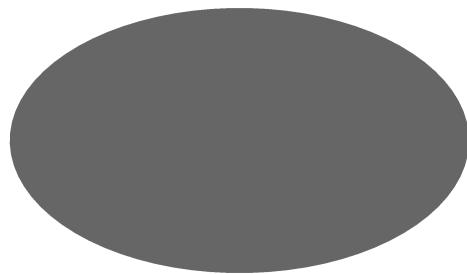
Figure 4.7: Notably higher mesh quality vertically for double cut sphere with WebMGA 2.0



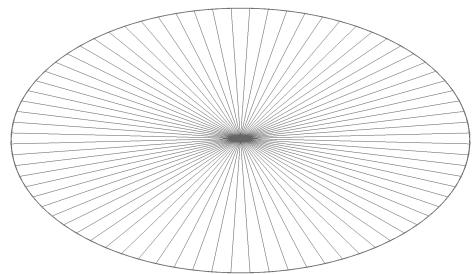
(a) WebMGA 2.0 Shape



(b) WebMGA 2.0 Wireframe



(c) WebMGA 3.0 Shape



(d) WebMGA 3.0 Wireframe

Figure 4.8: Buggy shape representation when double cut sphere has 0 height

surface in such a way as to split it into a finite number of flat, triangular sub-faces as shown in Figure 4.9. This sampling is performed with the spherical coordinates system for some sphere radius r , azimuthal angles θ , and polar angles ϕ , converted to an equivalent Cartesian form. A point in spherical coordinate space is denoted \mathbf{r}_s , while a point in Cartesian space is denoted \mathbf{r}_C ,

$$\mathbf{r}_s = \begin{pmatrix} r \\ \phi \\ \theta \end{pmatrix} \quad (4.3)$$

$$\mathbf{r}_C = \begin{pmatrix} r \sin \phi \cos \theta \\ r \sin \phi \sin \theta \\ r \cos \phi \end{pmatrix} \quad (4.4)$$

Any unique point on the origin centred r sphere can be uniquely defined by some (θ, ϕ) pair. Therefore, to evenly space points across the surface, a set of θ s and ϕ s is generated by taking n (essentially a measure of mesh quality) evenly spaced values over the interval of a full circular rotation ($[0, 2\pi]$). Each unique pairing (ϕ, γ) , along with r , is used to produce the full set of Cartesian vertices using Equation (4.4). This method is sufficient to produce a sphere mesh as in Figure 4.10a from WebMGA 2.0. The sampling is modified slightly for WebMGA 3.0 to produce a mesh as in Figure 4.10c by offsetting each row such that points on one row lie half way between a pair of points on the row above since it produces a slightly more visually satisfying mesh. The code was rewritten from scratch since most other shapes result from slight modifications to the sphere generation process, and the initial WebMGA 2.0 implementation was over-complicated and proved difficult to extend.

TODO DISCUSS ORDERIGN AND FACES ETC.

Some optimisations are implemented to efficiently generate a full set of vertices while sampling only $\frac{1}{4}$ of the points around the sphere's surface. This uses the fact that the origin centred sphere is symmetrical in each of the xy , xz , and yz planes. Points for the quarter sphere can be generated by applying Equation (4.4) with all pairings of $\frac{n}{2}$ evenly spaced $\theta \in [0, \pi]$, and $\frac{n}{2}$ evenly spaced $\phi \in [0, \frac{\pi}{2}]$. These points are arranged in a 3d array corresponding to rows (from ϕ) and columns (from θ).

An additional set of points for the diagonally opposite quarter is trivially generated with correct vertex ordering by copying the original quarter vertices and negating the x and y values for each vertex to mirror in the xz and yz planes. TODO FINISH

TODO OPTIMISATION DIAGRAM

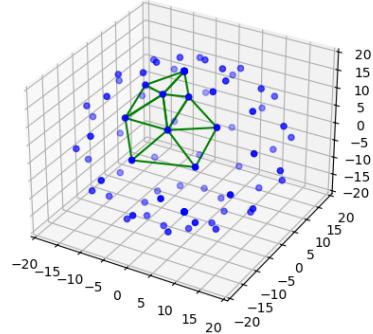


Figure 4.9: Example sphere vertex distribution (9×10 vertical \times horizontal samples). Some mesh edges shown to demonstrate mesh construction from vertices.

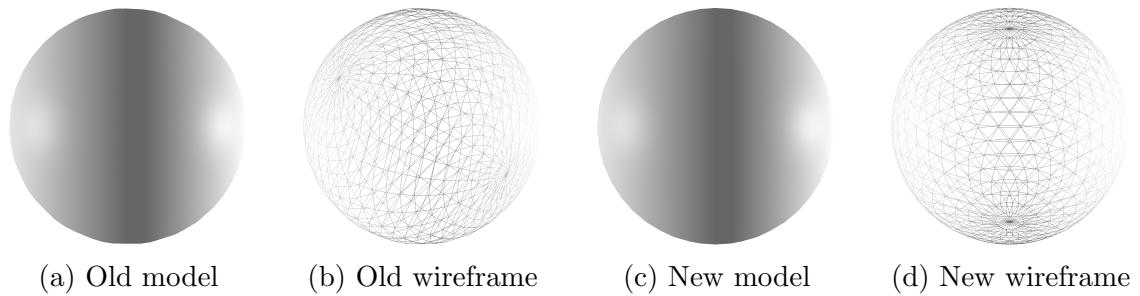


Figure 4.10: Sphere molecule mesh implementation.

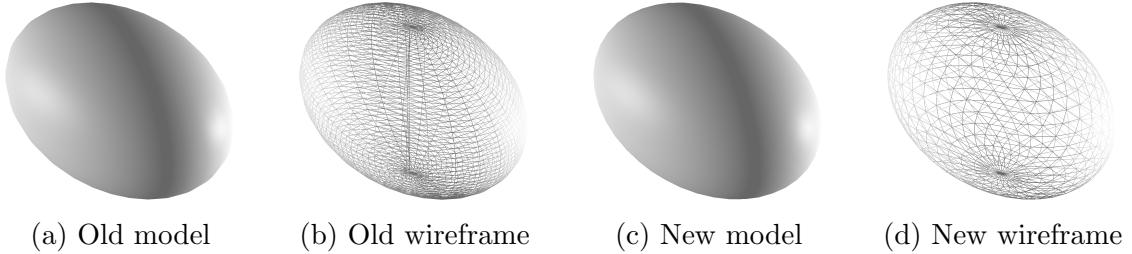


Figure 4.11: Ellipsoid molecule mesh implementation.

Ellipsoid

The ellipsoid shape (Figure 4.11, parameters “X”, “Y”, “Z”) can be represented as an origin centred sphere of radius 1 scaled in the x,y and z directions by some scalar value in each direction. This can be represented by a slightly modified form of the Cartesian sphere equation in Equation (4.4), where \mathbf{S} denotes some scaling vector,

$$\mathbf{r}_e = \begin{pmatrix} s_x r \sin \phi \cos \theta \\ s_y r \sin \phi \sin \theta \\ s_z r \cos \theta \end{pmatrix} = \mathbf{S} \odot \mathbf{r}_C \quad (4.5)$$

. From this formulation, it can be seen that an ellipsoid can be generated by slightly modifying the vertex sampling process for a sphere, whilst leaving the rest of the mesh building process unchanged. A sphere point can be sampled using Equation (4.4) with radius 1 and then multiplied by the scaling vector $(s_x, s_y, s_z)^T$ to give an equivalent result to Equation (4.5).

In the program this is implemented by creating an “Ellipsoid” class as a child of the “Sphere” class and overriding the “sample_sphere()” method. Since this implementation is so simple, the JavaScript code is provided below:

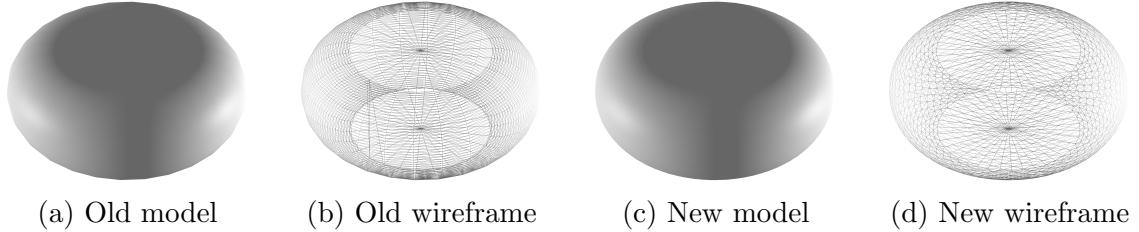


Figure 4.12: Spheroplatelet molecule mesh implementation.

```
// Ellipsoid mesh generator
export class Ellipsoid extends Sphere {
    // Scale factor in [x, y, z] directions
    scale: number [];

    constructor(x: number, y: number, z: number) {
        // Derive from origin centred sphere of radius 1
        super(1);
        this.scale = [x, y, z];
    }

    // Samples from ellipsoid instead of sphere
    sampleSphere(radius: number, theta: number, phi: number): number [] {
        // Multiply origin centred sphere coordinates by scale vector
        return math.dotMultiply(super.sampleSphere(radius, theta, phi), this.scale);
    }
}
```

Spheroplatelet

The spheroplatelet shape (Figure 4.12, parameters “RadSphere” and “RadCircle”) is generated by modifying a generates sphere mesh (see Section 4.3.4). Vertices are iterated over and pushed outwards by applying to the below formula, following on from Equation (4.4) with c representing “RadCircle”, \mathbf{n} representing the sphere vertex normal in the x, y plane, and \mathbf{r}_p representing a vertex coordinate,

$$\mathbf{n} = \begin{pmatrix} r_x \\ r_y \end{pmatrix} \quad (4.6)$$

$$\mathbf{r}_p = \mathbf{r}_C + \frac{c\mathbf{n}}{\|\mathbf{n}\|_2}. \quad (4.7)$$

This will leave an empty circle of points at the top and bottom of the transformed geometry which can be filled by generating an additional vertices at the top and bottom respectively by averaging the coordinates for each vertex on the corresponding circle’s edge, splitting it into triangles. This can be observed on Figure 4.12d.

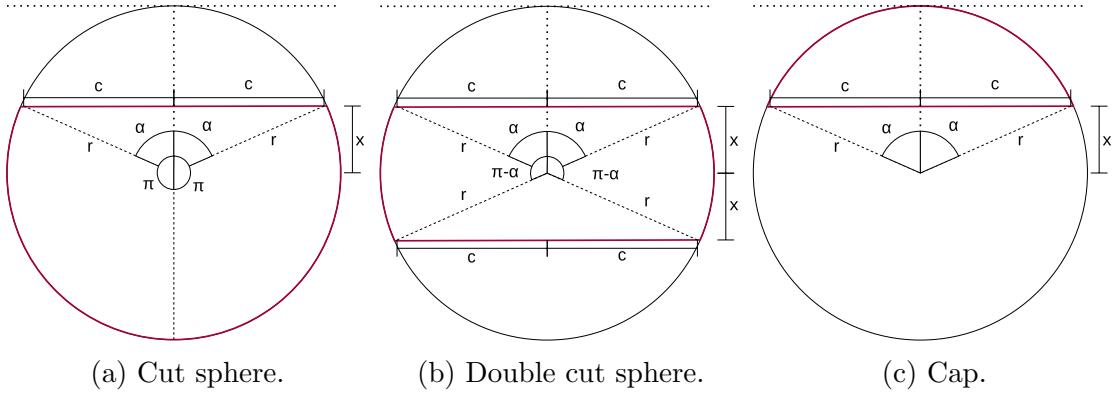


Figure 4.13: Cap and cut sphere shape diagrams. Lens outlines are shown by a red line, black lines demonstrate construction.

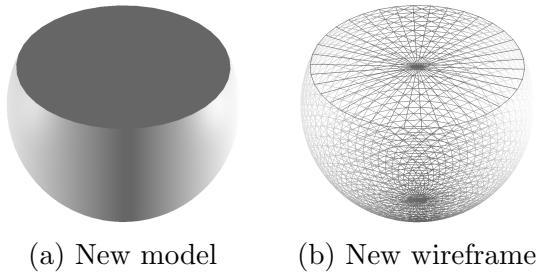


Figure 4.14: Cut sphere

Cut Sphere

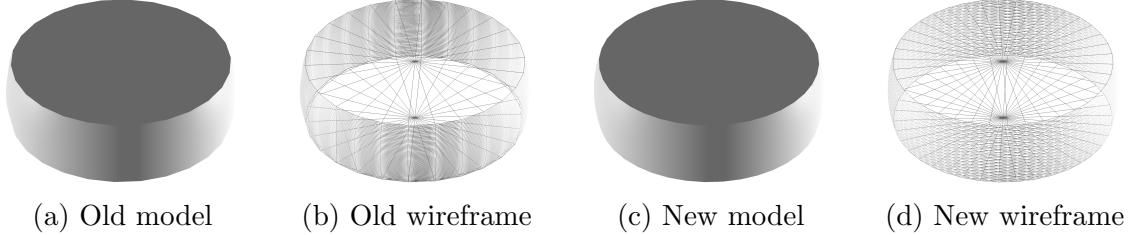
The cut sphere shape (Figure 4.14, parameters “Radius”, “zCut”) is implemented simply by sampling the sphere as before but over a reduced range of ϕ values. Since the sphere will not be completed, an empty circular face is left which can be filled by generating an additional vertex by averaging the coordinates for each vertex on the circle’s edge, splitting it into triangles. This can be observed on Figure 4.14b.

A cut sphere is parameterised in WebMGA using a parent sphere radius and a zCut distance. These are shown in Figure 4.13a, with characters r and x respectively. The new range of ϕ s can be seen in the diagram as the range $[\alpha, \pi)$, which can be reinterpreted in terms of r and x as follows,

$$\alpha = \arcsin \frac{c}{r} \quad (4.8)$$

$$c = \sqrt{r^2 - x^2} \quad (4.9)$$

$$[\alpha, \pi) = [\arcsin \frac{c}{r}, \pi) \quad (4.10)$$



(a) Old model (b) Old wireframe (c) New model (d) New wireframe

Figure 4.15: Double cut sphere molecule mesh implementation.

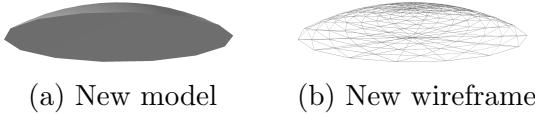


Figure 4.16: Cap

Double Cut Sphere

The double cut sphere shape (Figure 4.15, parameters “Radius”, “zCut”) is implemented simply by sampling the sphere as before but over a reduced range of ϕ values. Since the sphere will not be completed, two empty circular faces are left which can be filled by generating two additional vertices by averaging the coordinates for each vertex on the corresponding circle’s edge, splitting it into triangles. This can be observed on Figure 4.15d.

A double cut sphere is parameterised in WebMGA using a parent sphere radius and a zCut distance. These are shown in Figure 4.13b, with characters r and x respectively. The new range of ϕ s can be seen in the diagram as the range $[\alpha, \pi - \alpha)$, which can be reinterpreted in terms of r and x as follows,

$$\alpha = \arcsin \frac{c}{r} \quad (4.11)$$

$$c = \sqrt{r^2 - x^2} \quad (4.12)$$

$$[\alpha, \pi - \alpha) = [\arcsin \frac{c}{r}, \pi - \arcsin \frac{c}{r}) \quad (4.13)$$

Cap

The cap shape (Figure 4.16, parameters “Radius”, “zCut”) is implemented simply by sampling the sphere as before but over a reduced range of ϕ values. Since the sphere will not be completed, an empty circular face is left which can be filled by generating an additional vertex by averaging the coordinates for each vertex on the circle’s edge, splitting it into triangles. This can be observed on Figure 4.16b.

A cap is parameterised in WebMGA using a parent sphere radius and a zCut distance.

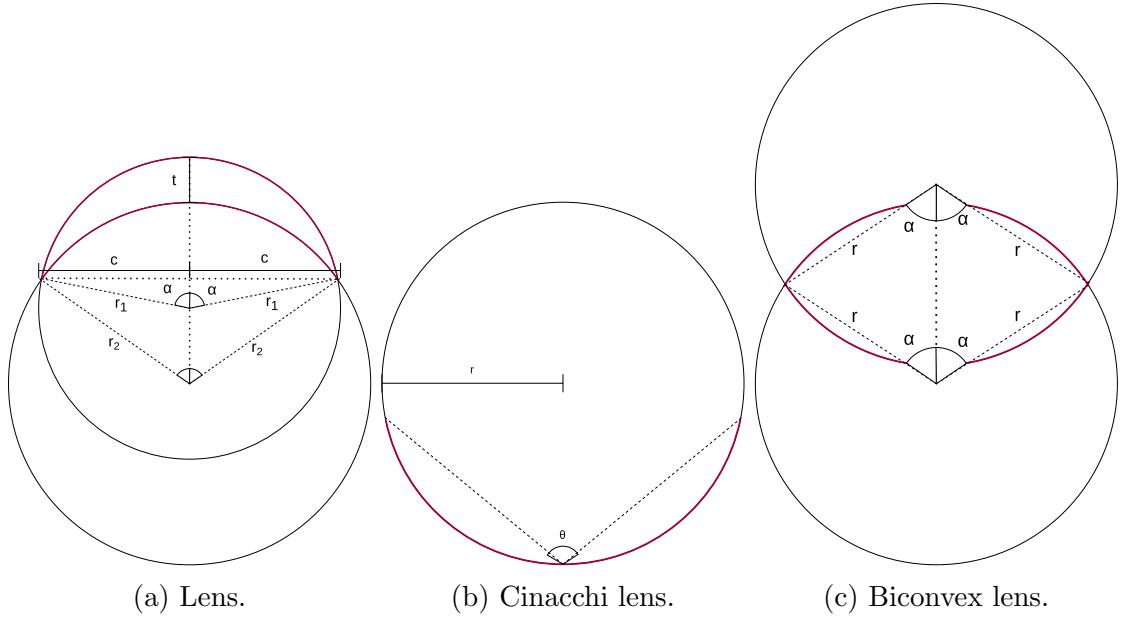


Figure 4.17: Lens shape diagrams. Lens outlines are shown by a red line, black lines demonstrate construction.

These are shown in Figure 4.13c, with characters r and x respectively. The new range of ϕ s can be seen in the diagram as the range $[0, \alpha]$, which can be reinterpreted in terms of r and x as follows,

$$\alpha = \arcsin \frac{c}{r} \quad (4.14)$$

$$c = \sqrt{r^2 - x^2} \quad (4.15)$$

$$[0, \alpha] = [0, \arcsin \frac{c}{r}] \quad (4.16)$$

Lens

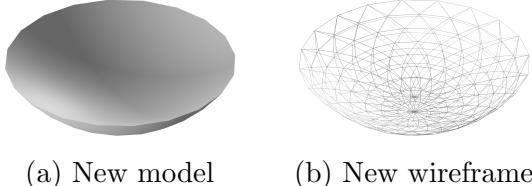
The lens shape (Figure 4.18, parameters “Radius”, “Thickness”, “Angle”) is created by assembling either two caps (Section 4.3.4) or a cap and a cut sphere (Section 4.3.4) to recreate the format shown in Figure 4.17a. For the upper part of the lens, a cap is generated with angle parameter α . For the lower part of the lens, if the required θ is greater than $\frac{\pi}{2}$ then a TODO FINISH

Base Lens

Thick Lens

Cinacchi Lens

During development, some sample configurations requiring the lens molecule shape were provided by Giorgio Cinacchi. This is named the “Cinacchi Lens” in WebMGA (param-



(a) New model (b) New wireframe

Figure 4.18: Lens

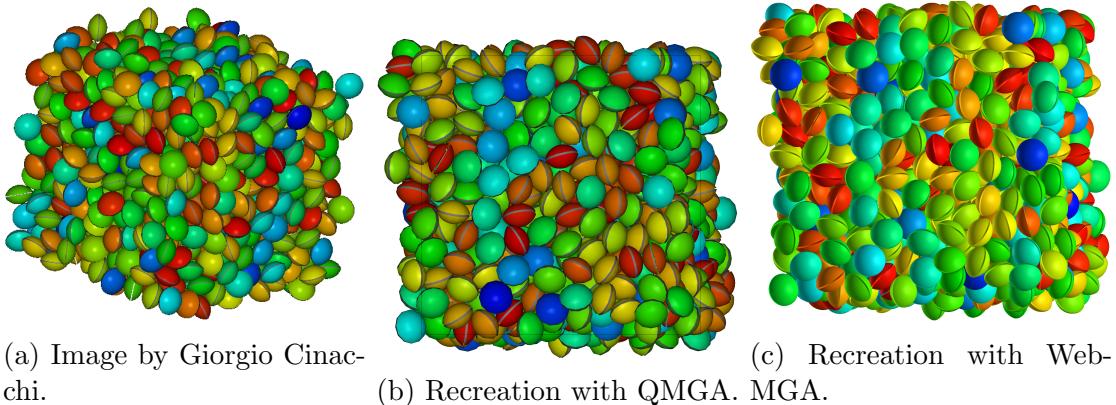


Figure 4.19: Lens setup required by Giorgio Cinacchi.

eters “Radius”). For these configurations, Cinacchi uses a specific lens configuration as shown in Figure 4.17b which is parameterised using only a single r value,

$$\cos \theta = 1 - \frac{1}{2\pi r^2} \quad (4.17)$$

$$\theta = \arccos \left(1 - \frac{1}{2\pi r^2} \right). \quad (4.18)$$

This produces an infinitely thin lens with some aperture angle dependent on the radius. The Cinnachi lens is implemented simply as a parameterisation of the base lens in Section 4.3.4 where the two radii are both r , and the angle is derived from Equation (4.18).

A screenshot produced using QMGA was provided by Cinacchi to assist in visually verifying the shape produced. This is shown in Figure 4.19a. A recreation was produced in QMGA as shown in Figure 4.19b, then WebMGA as shown in Figure 4.19c. This appears to verify a correct implementation.

Biconvex Lens

Spherocylinder

The spherocylinder shape (Figure 4.21, parameters “Radius”, “Length”) can be represented as an origin centred sphere of radius r scaled in the z directions by (half of) some length value in each z direction (positive/negative). This can be represented by a slightly

modified form of the Cartesian sphere equation in Equation (4.4),

$$\mathbf{r}_c = \begin{pmatrix} r \sin \phi \cos \theta \\ r \sin \phi \sin \theta \\ r \cos \theta + n \end{pmatrix} = \mathbf{r}_C + \begin{pmatrix} 0 \\ 0 \\ n \end{pmatrix} \quad (4.19)$$

$$n = \begin{cases} \frac{\text{length}}{2} & \text{if } r \cos \theta > 0 \\ -\frac{\text{length}}{2} & \text{if } r \cos \theta < 0 \\ 0 & \text{otherwise.} \end{cases} \quad (4.20)$$

Initial Attempt From Equations (4.19) and (4.20), it can be seen that a spherocylinder can be approximated by slightly modifying the vertex sampling process for a sphere, whilst leaving the rest of the mesh building process unchanged. A sphere point can be sampled using Equation (4.4) with radius r and added to the scaling vector $(0, 0, n)^T$ as defined in Equation (4.20) to give an equivalent result to Equation (4.19).

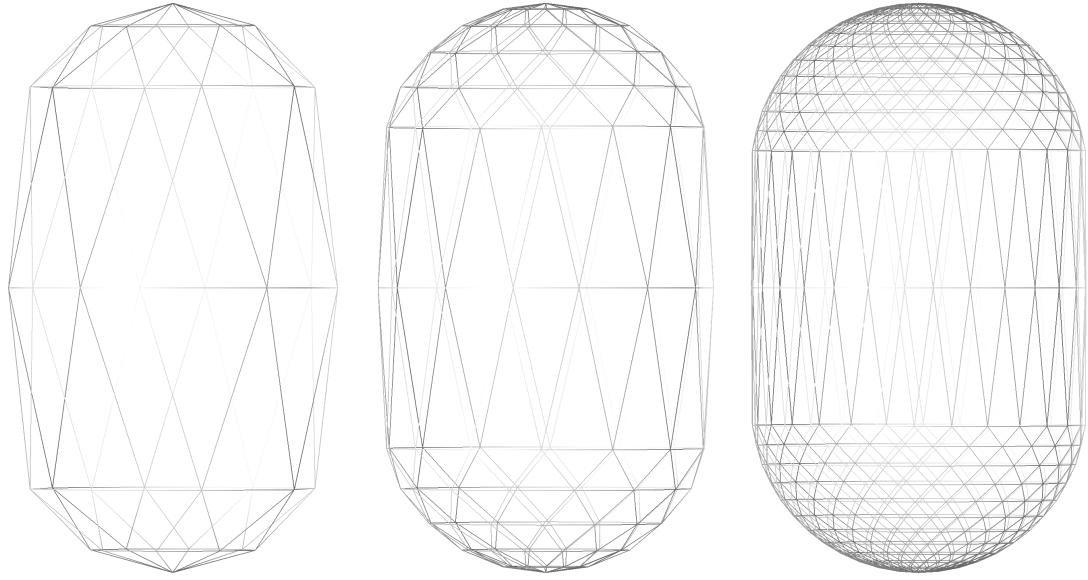
In the program this was implemented by creating a “Spherocylinder” class as a child of the “Sphere” class and overriding the “sample_sphere()” method. Since this implementation is so simple, the JavaScript code is provided below:

```
//Spherocylinder mesh generator
export class Spherocylinder extends Sphere {
    //Scaling vector (either side of centre) to stretch sphere into spherocylinder ([0, 0, length / 2])
    length_scaling_vector: number[];

    constructor(radius: number, length: number) {
        //Derive from origin centred sphere of chosen radius
        super(radius);
        this.length_scaling_vector = [0, 0, length / 2];
    }

    //Samples from spherocylinder instead of sphere
    sample_sphere(radius: number, theta: number, phi: number, epsilon: number = 1e-15): number[] {
        let sphere_coordinate: number[] = super.sample_sphere(radius, theta, phi);
        //Stretch point in z direction by scale vector, matching stretch direction to sign of original vertex z
        //Unchanged if z is (approximately) 0
        if (Math.abs(sphere_coordinate[2]) < epsilon) {
        } else if (sphere_coordinate[2] > 0) {
            sphere_coordinate = math.add(sphere_coordinate, this.length_scaling_vector);
        } else if (sphere_coordinate[2] < 0) {
            sphere_coordinate = math.subtract(sphere_coordinate, this.length_scaling_vector);
        }
        return sphere_coordinate;
    }
}
```

Unfortunately, this process produced visually unsatisfying results with the sides of the spherocylinder visibly tapering, particularly with low detail meshes. This can be seen in Figure 4.20. After producing the biconvex lens (Section 4.3.4), an alternate, much simpler solution became apparent which avoided this issue.



(a) Low mesh density. (b) Medium mesh density. (c) High mesh density.

Figure 4.20: Initial spherocylinder implementation. Visible tapering can be observed, particularly with low mesh density.

Second Attempt A spherocylinder can also be considered a special case of the biconvex lens. A biconvex lens with no separation and aperture angle $\frac{\pi}{2}$ produces a sphere with the given radius r . Increasing the separation parameter causes the two hemispheres to move apart such that a spherocylinder is produced. The spherocylinder can therefore simply be considered a special case of the biconvex lens with aperture angle $\frac{\pi}{2}$, and can be implemented entirely through class inheritance as shown:

```
//Spherocylinder mesh generator
export class Spherocylinder extends BiconvexLens {
    constructor(radius: number, length: number) {
        super(radius, Math.PI / 2, length);
    }
}
```

This produced the result shown in Figure 4.21.

4.3.5 WebMGA 3.0 Bugs

TODO

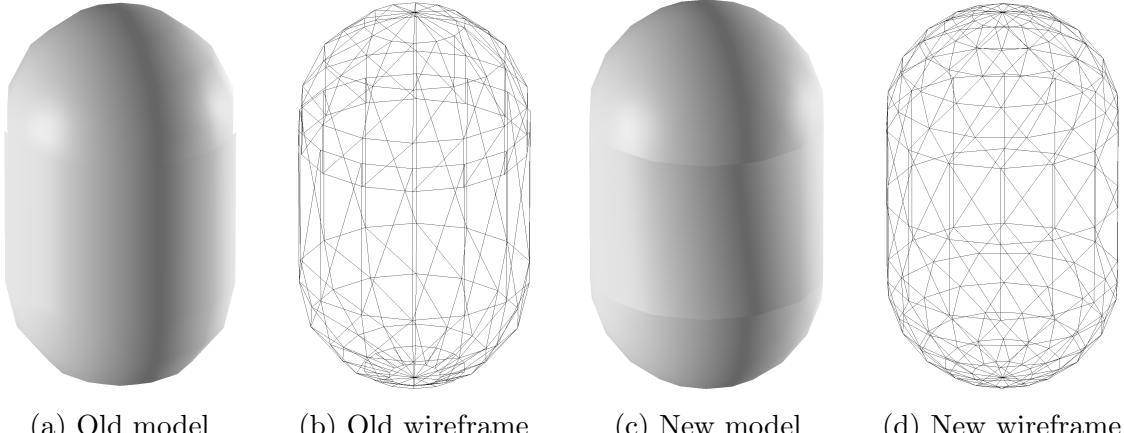


Figure 4.21: Spherocylinder molecule mesh implementation.

4.4 File types

4.4.1 WebMGA 2.0 Implementation

WebMGA 2.0 supports only its own JSON-based file format as defined by Battistini. This could prove an obstacle to users since, in practice, different formats are output when running molecular dynamics simulations (CITE!!).

4.4.2 WebMGA 2.0 Bugs

TODO

4.4.3 WebMGA 3.0 Implementation

WebMGA 3.0 implements two new file formats for defining molecular configurations as defined below.

CNF (LAMMPS) Format (.cnf)

LAMMPS is a molecular dynamics simulator typically used on highly parallel computers[19]. It uses a specifically designed file format to represent molecular configurations to allow the highest possible performance while preserving some amount of human readability.

Table 4.1 shows the structure of a file of this format. Rows represent lines in the file. Each value is represented by a signed float of format -1.000000 , where digits before the decimal are omitted if not present. Values are separated by spaces, padded to align decimal points.

For WebMGA 3.0, a parser script was written in JavaScript which builds a WebMGA JSON configuration from the “.cnf” file provided. Specifically, a unit box is constructed

Molecule count											
Unit box X length (lx)											
Unit box Y length (ly)											
Unit box Z length (lz)											
Not used	Not used										
Position (rx)	Position (ry)	Position (rz)	Velocity (vx)	Velocity (vy)	Velocity (vz)	Orientation (ex)	Orientation (ey)	Orientation (ez)	Orientational velocity (ux)	Orientational velocity (uy)	Orientational velocity (uz)
:	:	:	:	:	:	:	:	:	:	:	:
											Molecule ID

Table 4.1: CNF format molecule configuration.

Unit box X half length ($lx/2$)	Unit box Y half length ($ly/2$)	Unit box Z half length ($lz/2$)								
Shape parameter	Position X (rx)	Position Y (ry)	Position Z (rz)	Orientation X (ex)	Orientation Y (ey)	Orientation Z (ez)				
:	:	:	:	:	:	:				

Table 4.2: Cinacchi format molecule configuration.

from (lx, ly, lz) , and molecule positions and orientations are obtained from corresponding pairs of $((rx, ry, rz), (ex, ey, ez))$ for some molecule id. All other parameters are dropped since they aren't used by WebMGA. Molecules are ordered in an array according to their id.

Cinacchi Format (.qmga)

TODO WRITE THIS TODO CHECK LETTERS USED FOR ROTATION ETC

See Table 4.2 for the structure of a file of this format. Rows represent lines in the file. Each value is represented by a signed float of format -1.00000000 , where digits before the decimal are omitted if not present. Values are separated by spaces, padded to align decimal points.

For WebMGA 3.0, a parser script was written in JavaScript which builds a WebMGA JSON configuration from the “.qmga” file provided. Specifically, a unit box is constructed from (lx, ly, lz) , and molecule positions and orientations are obtained from corresponding pairs of $((rx, ry, rz), (ex, ey, ez))$. The shape parameter is dropped since molecule shape is not defined by the file. Molecules are ordered in an array as they are encountered.

4.4.4 WebMGA 3.0 Bugs

WebMGA ignores the shape parameter from the “.qmga” format configuration. Since some shapes in WebMGA require multiple parameters, and the shape to use is not defined within the file, I could not see a sensible way to automate applying this. The user must manually enter this value after selecting a molecule shape in the “Models” menu. This is not ideal since a user should expect their configuration to appear correctly as soon as they load the file.

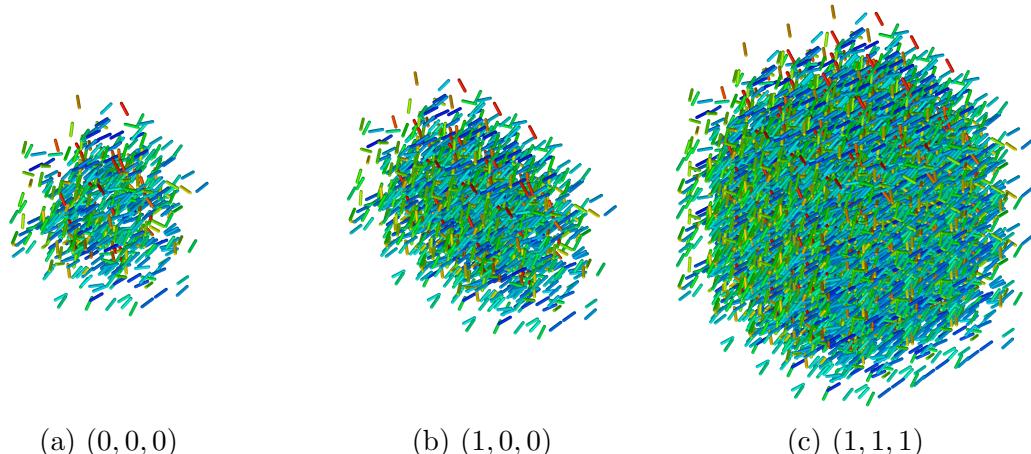


Figure 4.22: Demonstration of periodic repetition of a configuration, labelled with repetition parameter of format (x, y, z) .

4.5 Periodic Repetition

4.5.1 Improvement Goals

A description for periodic boundary conditions is given in Section 2.2.2 regarding how a small simulation box simulates a subset of an infinite lattice. It may be useful to visualise a larger subset of this infinite lattice by repeating the simulation box a number of times. Additionally, the capability of repeating a smaller system is useful for producing a realistic, much larger configuration for testing the performance of WebMGA with increased molecule counts due to the lack of availability of real test configurations of such sizes.

4.5.2 WebMGA 3.0 Implementation

A few modifications needed to be made to implement this feature.

First, the “reference” tab in the side menu was modified to include inputs for the repeat count in the ‘x’ ‘y’ and ‘z’ directions. With a value of zero, there should be only a single instance of the configuration along the corresponding axis. Setting to one adds a repeat in the positive and negative direction along the axis, with bounding box faces touching (i.e. with a value of 0, there will be 1 instance of the configuration, with 1 there will be 3 instances, 2 there will be 5 instances etc.). When multiple directions have a value larger than 0, the configurations are repeated such that a single large box is produced (i.e. it is ensured there are no gaps, for example a configuration of (1, 1, 1) will give a box of dimensions $3 \times 3 \times 3$ with 27 total instances of the initial configuration).

Repetition of the configuration was implemented by changing TODO FINISH THIS

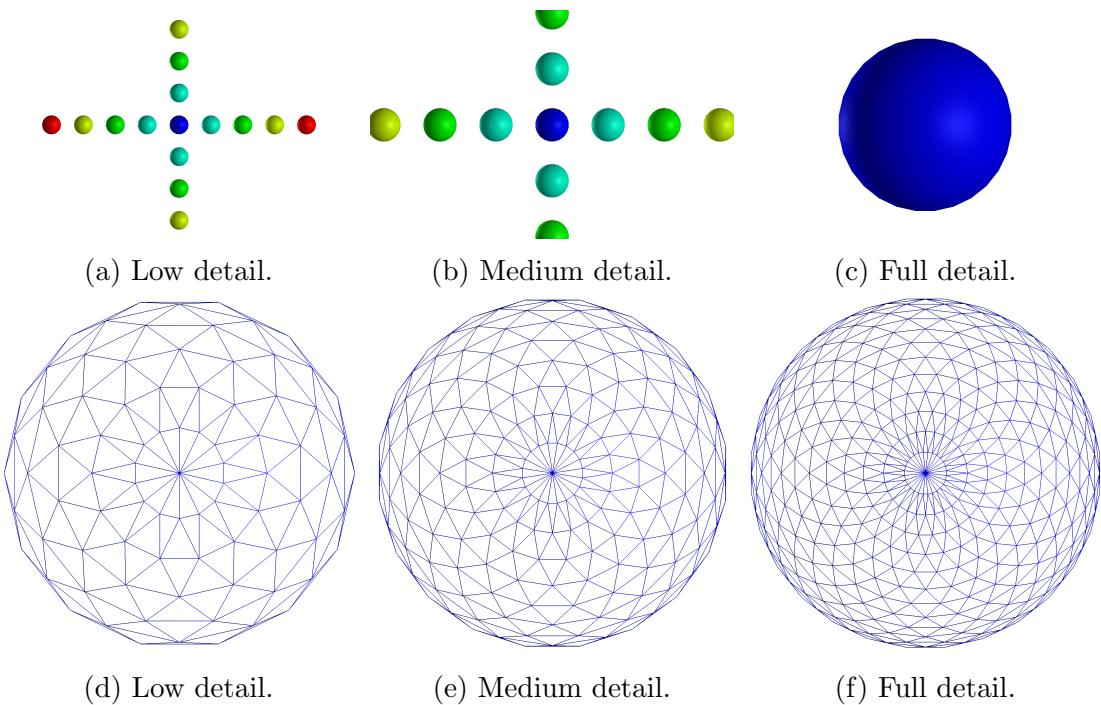


Figure 4.23: Model complexity is decreased at subjectively chosen camera distance thresholds with minimal visible loss in quality.

4.5.3 WebMGA 3.0 Bugs

TODO

4.6 Optimisations

4.6.1 WebMGA 2.0 Implementation

TODO

4.6.2 WebMGA 2.0 Bugs

TODO

4.6.3 WebMGA 3.0 Implementation

Discrete Levels of Detail

Performance analysis for this optimisation is discussed in Section 5.1.

4.6.4 WebMGA 3.0 Bugs

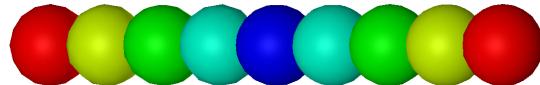
TODO



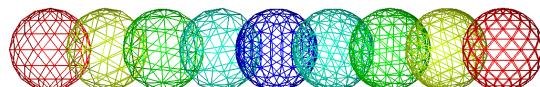
(a) At a similar distance, all objects are identical.



(b) At a similar distance, all meshes are identical.



(c) Further spheres have a minor decrease in visible quality.



(d) Further spheres have a minor decrease in triangle density.

Figure 4.24: Demonstration of decreased mesh quality for distant object. “Level of Detail” setting has been reduced below default for a more visible geometry reduction.

4.7 Miscellaneous Improvements

Chapter 5

Analysis and Testing

5.1 Level of Detail Performance

5.2 Configuration Visualisations

LOD Enabled	Mesh Quality	Repeats	Distant Framerate (7)	Nearby Framerate (50)	Nearest Framerate (100)
True	High	(0, 0, 0)	48.6	26.4	22.2
False	High	(0, 0, 0)	2.4	1.2	0.6
True	Default	(0, 0, 0)	36.6	27.6	21.0
False	Default	(0, 0, 0)	14.4	4.8	1.2
True	Low	(0, 0, 0)	32.4	28.2	22.8
False	Low	(0, 0, 0)	16.2	8.4	3.0
True	High	(1, 1, 1)	9.64	8.43	10.54
False	High	(1, 1, 1)	0.86	1.87	3.97
True	Default	(1, 1, 1)			
False	Default	(1, 1, 1)			
True	Low	(1, 1, 1)			
False	Low	(1, 1, 1)			

Table 5.1: TODO TITLE. MENTION THERMAL THROTTLING ISSUES

Chapter 6

Conclusions and Evaluation

6.1 Achievements

Summarise the achievements to confirm the project goals have been met.

6.2 Evaluation

Evaluation of the work (this may be in a separate chapter if there is substantial evaluation).

6.3 Future Work

Bibliography

- [1] Eduardo Battistini. Webmga, 2021. URL: <https://students.cs.ucl.ac.uk/2019/group3/WebMGA/diss.pdf>.
- [2] Yue He. Webmga 2.0, 2023.
- [3] Adrian T Gabriel, Timm Meyer, and Guido Germano. Molecular graphics of convex body fluids. *Journal of Chemical Theory and Computation*, 4(3):468–476, 2008.
- [4] Webmga 3.0. URL: <https://joe-down.github.io/WebMGA-3>.
- [5] Webmga 3.0 github repository. URL: <https://github.com/joe-down/WebMGA-3>.
- [6] React. URL: <https://react.dev/>.
- [7] Three.js. URL: <https://threejs.org/>.
- [8] Qmga sourceforge.net. URL: <https://sourceforge.net/projects/qmga/files/qmga/>.
- [9] Juan Pedro Ramírez González and Giorgio Cinacchi. Densest-known packings and phase behavior of hard spherical capsids. *The Journal of Chemical Physics*, 159(4), 2023.
- [10] Valerio Mazzilli, Katsuhiko Satoh, and Giacomo Saielli. Phase behaviour of mixtures of charged soft disks and spheres. *Soft Matter*, 19(18):3311–3324, 2023.
- [11] Richard James, Eero Willman, FA FernandezFernandez, and Sally E Day. Finite-element modeling of liquid-crystal hydrodynamics with a variable degree of order. *IEEE Transactions on Electron Devices*, 53(7):1575–1582, 2006.
- [12] Lcview. URL: <https://www.ee.ucl.ac.uk/~afernand/rjames/modelling/visualisation/>.
- [13] Qt 3 debian removal. URL: <https://wiki.debian.org/qt3-x11-freeRemoval>.
- [14] Michael P Allen and Dominic J Tildesley. *Computer simulation of liquids*. Oxford university press, 2017.
- [15] Ronald Y Dong and Ronald Y Dong. Orientational order. *Nuclear Magnetic Resonance of Liquid Crystals*:53–89, 1997.

- [16] Weidong Wu, Joseph Owino, Ahmed Al-Ostaz, and Liguang Cai. Applying periodic boundary conditions in finite element analysis. In *SIMULIA community conference, Providence*, pages 707–719, 2014.
- [17] Michael P Allen. Molecular simulation of liquid crystals. *Molecular Physics*, 117(18):2391–2417, 2019.
- [18] Giorgio Cinacchi and Salvatore Torquato. Hard convex lens-shaped particles: characterization of dense disordered packings. *Physical Review E*, 100(6):062902, 2019.
- [19] Aidan P Thompson, H Metin Aktulga, Richard Berger, Dan S Bolintineanu, W Michael Brown, Paul S Crozier, Pieter J In’t Veld, Axel Kohlmeyer, Stan G Moore, Trung Dac Nguyen, et al. Lammps-a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Computer Physics Communications*, 271:108171, 2022.

Appendix A

Appendices

A.1 Project proposal

Project Plan

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

Joe Down

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
- g.germano@ucl.ac.uk

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. back-face 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 foresee 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.

A.2 Interim Report

Interim Report

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

Joe Down

January 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
- g.germano@ucl.ac.uk

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 factor 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