Simulating 3 dimensional Smectic Liquid Crystals

Djordje Mihajlovic

Edinburgh University

Liquid Crystals

Liquid crystals are a type of mesophase - a state of matter exhibiting both liquid and crystalline properties.

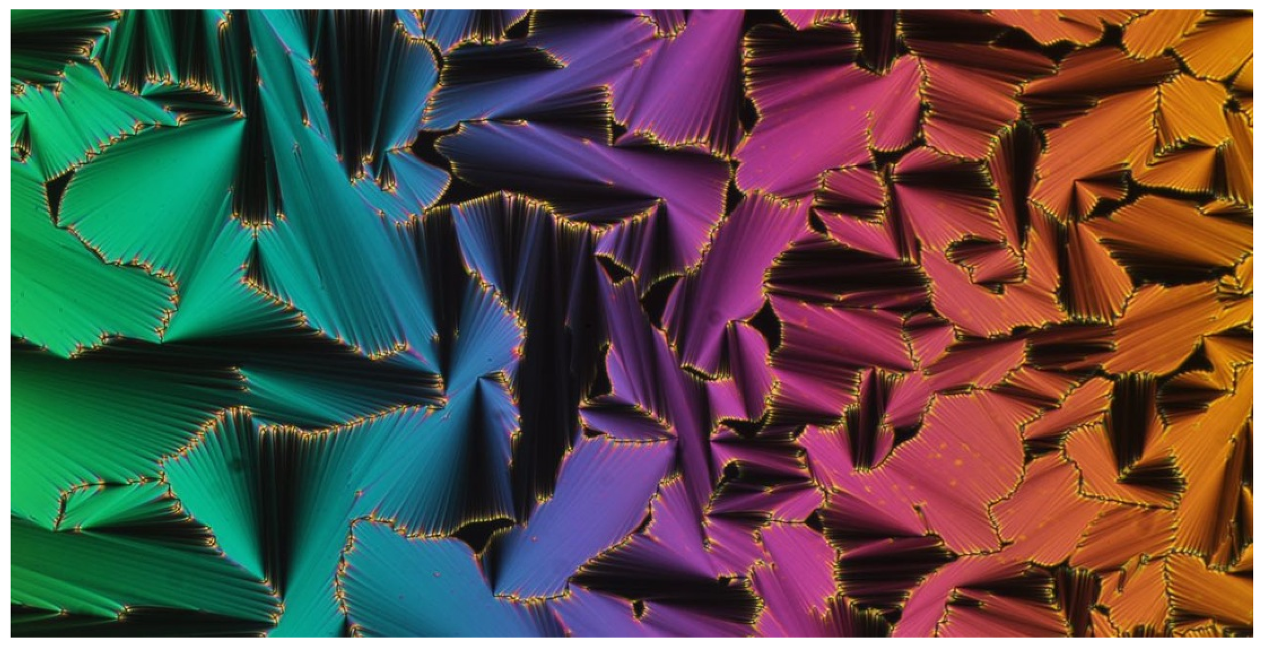

Figure 1. Smectic A liquid crystal [1].

These properties arise as a result of the specific ordering that occurs in a liquid crystal. Similar to a crystal, liquid crystal phases have orientational and/or translational order. However, this order is limited in dimension, therefore allowing the phase of matter to exhibit both liquid and crystalline behaviour.

The smectic phase

A specific type of liquid crystal phase of interest is the smectic phase. The smectic phase exhibits both orientational order (the molecules tend to align to some normal) and translational order (the molecules form layers).

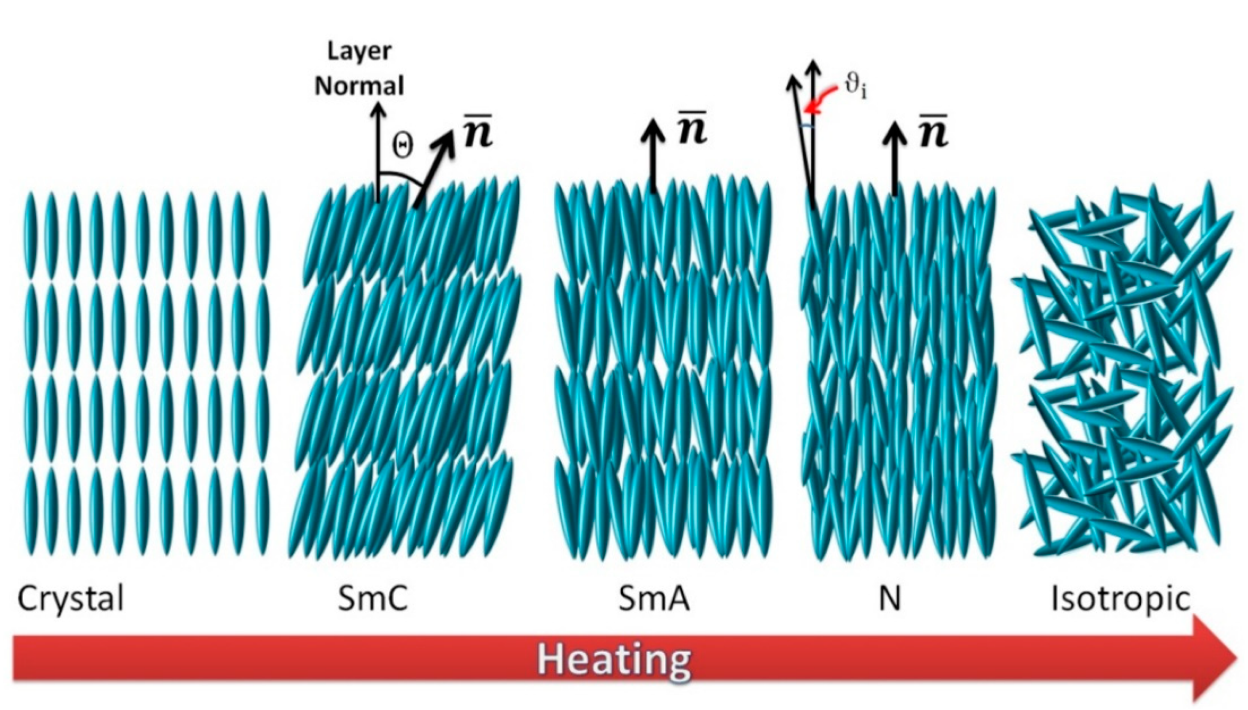

Figure 2. Different liquid crystal phases [2].

Mathematical modelling of smectics

Based on the priorly successful Q-tensor theory by De-Gennes, the smectic $\underline{\underline{E}}$-tensor was devised to mathematically model the smectic liquid crystal phase [3].

$$\underline{\underline{E}}(\underline{r},t) = |\psi|\, e^{i\phi}(\underline{N} \otimes \underline{N} - \frac{\delta}{d}) \tag{1}$$

Properties of the smectic $\underline{\underline{E}}$-tensor

The equation

$$\mu\frac{\partial E_{ij}}{\partial t} = -\frac{\delta F}{\delta E^*_{ij}} + \Lambda_{ij} \tag{2}$$

dictates how the $\underline{\underline{E}}$-tensor evolves according to a free energy F. The Λ_{ij} term is a Lagrange multiplier added to ensure certain properties of the E tensor are upheld. Specifically, the constraints on which the Lagrange multiplier is built are

$$g_1 = E_{ii} = 0 \tag{3}$$

$$g_2 = \frac{1}{2}tr([\underline{\underline{E}}, \underline{\underline{E}}^*]^2) \tag{4}$$

Originally a Lagrange multiplier was devised and implemented into the simulation for 2 dimensions, however due to its form does not work in the 3 dimensional case and fails to constrain a consistent 'complex phase' for each of the tensors components.

Simulations in 2D

With the constraints imposed via a Lagrange multiplier, 2-dimensional simulations can be run.

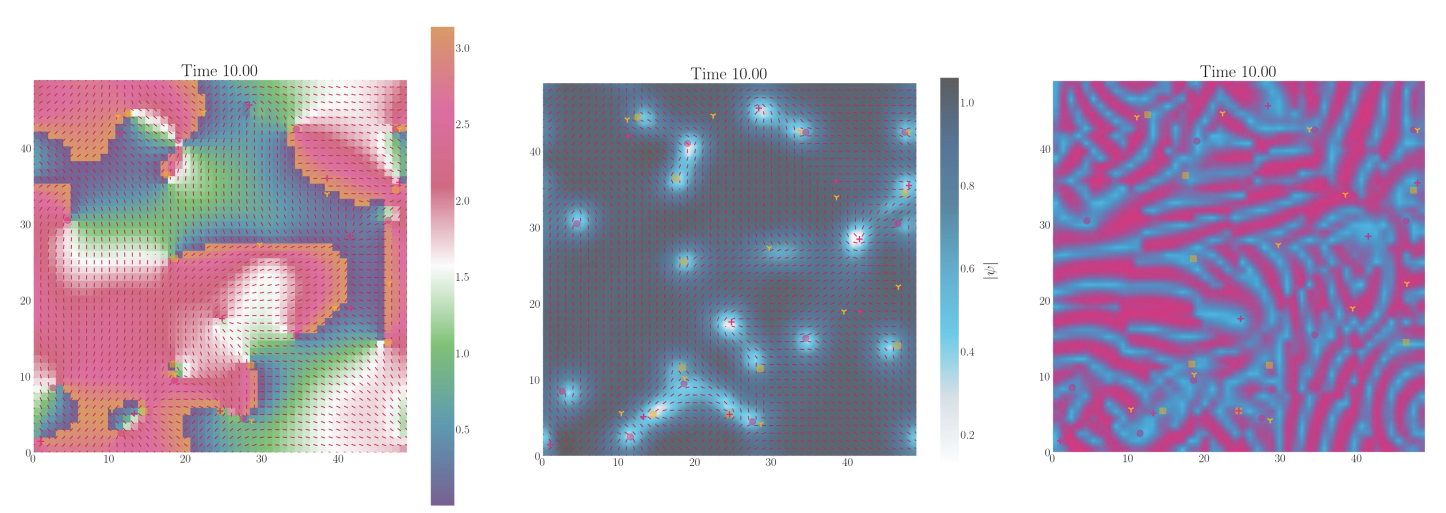

Figure 3. Periodic boundary condition smectic phase simulation after 10 second evolution. ϕ plot (right), $|\psi|$ plot (middle) and $Re\Psi$ plot (right), showing regional amount of dilation, ordering and layering respectively.

Lagrange Multiplier for 3 dimensions

Using a new constraint (equation 5), replacing g_2 (equation 4),

$$g_3 = [\underline{\underline{E}}, \underline{\underline{E}}^*] \odot [\underline{\underline{E}}, \underline{\underline{E}}^*] \tag{5}$$

A new Lagrange multiplier can then be derived of the form

$$\Lambda_{ij} = \delta_{ij}(\lambda_{1a} + i\lambda_{1b}) + \lambda_2\frac{\partial g_3}{\partial E^*_{ij}} \tag{6}$$

Where

$$\lambda_{1a} = \frac{\partial F}{\partial X_{ii}} - \lambda_2\frac{\partial g_3}{\partial X_{ii}}, \lambda_{1b} = \frac{\partial F}{\partial Y_{ii}} - \lambda_2\frac{\partial g_3}{\partial Y_{ii}} \tag{7}$$

$$\lambda_2 = \frac{c_1}{c_4} \tag{8}$$

X_{ij} and Y_{ij} represent the real and imaginary parts of the $\underline{\underline{E}}$-tensor, and c_1 and c_4 another set of derived partial differential equations.

Implementation and analysis

To analyse the implementation of the new Lagrange multiplier, the evolution of the complex phase of the tensor was plotted with and without the new Lagrange multiplier.

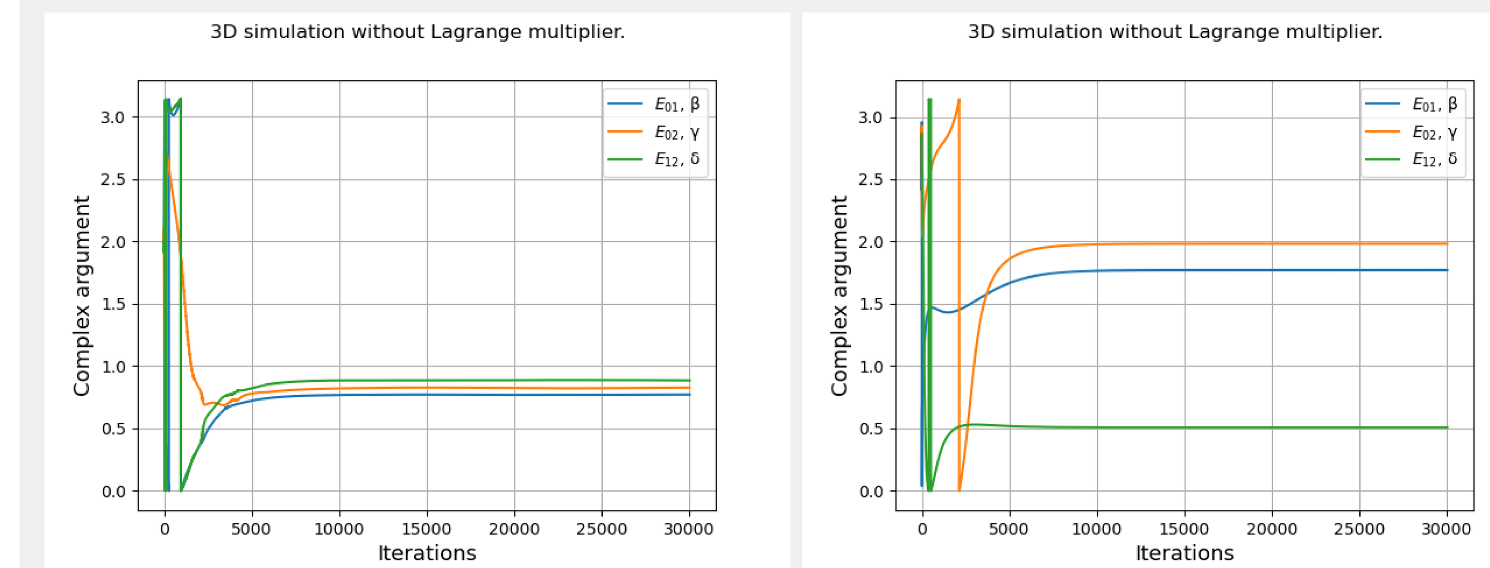

Figure 4. Plots of evolution of complex argument of $\underline{\underline{E}}$-tensor components with Lagrange multiplier (right) vs. without (right)

Further, to test that the action of the Lagrange multiplier was not altering the evolution of the tensors components past a local minima, i.e. constraining the components to have same complex phase by taking all components to zero, a plot of the tensors components evolution over time was also plotted.

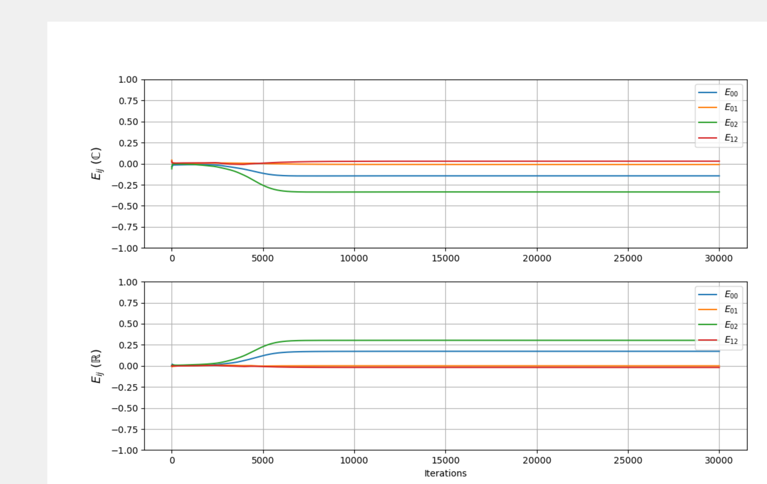

Figure 5. Evolution of imaginary (top) & real (bottom) values of components of the $\underline{\underline{E}}$-tensor.

Conclusion

The project set out to derive, implement and test a new Lagrange multiplier to ensure the evolution of the smectic $\underline{\underline{E}}$-tensor was consistent with the required constraints. A new Lagrange multipler was successfully derived and implemented, and subsequent tests were carried out. However, further tests can still be done to ensure the correct evolution of the tensors components.

References

[1] Vance Williams.
Liquid crystal microscopy.
`http://lcmicroscopy.weebly.com/lc-photogallery.html`.
Accessed: 2023-09-01.

[2] Zuhair Jamain, Ahmad Nor Asyraf Azman, Nurul Asma Razali, and Mohamad Zul Hilmey Makmud.
A review on mesophase and physical properties of cyclotriphosphazene derivatives with schiff base linkage.
Crystals, 12(8):1174, 2022.

[3] Jack Paget, Marco G Mazza, Andrew J Archer, and Tyler N Shendruk.
Complex-tensor theory of simple smectics.
Nature Communications, 14(1):1048, 2023.

[4] Claude E. Shannon.
A mathematical theory of communication.
Bell System Technical Journal, 27(3):379–423, 1948.

s1910360@ed.ac.uk