

# 3D Liquid Crystal Device Modelling

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## Q-LCsolver

### Program Description

The package comprises two modules; the modelling program and the visualisation package.

The modelling program calculates the dynamic evolution of the orientation of a liquid crystal material within a containing structure, subjected to time-varying voltages applied at electrodes. The containing structure can be of arbitrary shape. In the two-dimensional mode, this is a

cross-section while in the three-dimensional mode, it is a full cell, and can contain curved surfaces and protrusions.

A tensor formulation is the basis for the model, allowing for changes in the degree of order of the liquid crystal as well as for local biaxial ordering. This representation, in conjunction with adaptive meshing and adaptive time stepping in a

stable time integration scheme, allow for the accurate simulation of small scale features, such as defects, and their associated trajectories within relatively large container sizes. Also included in the model is an accurate treatment of the flow of the liquid crystal as well as anisotropic weak anchoring and the flexo-electric effect.

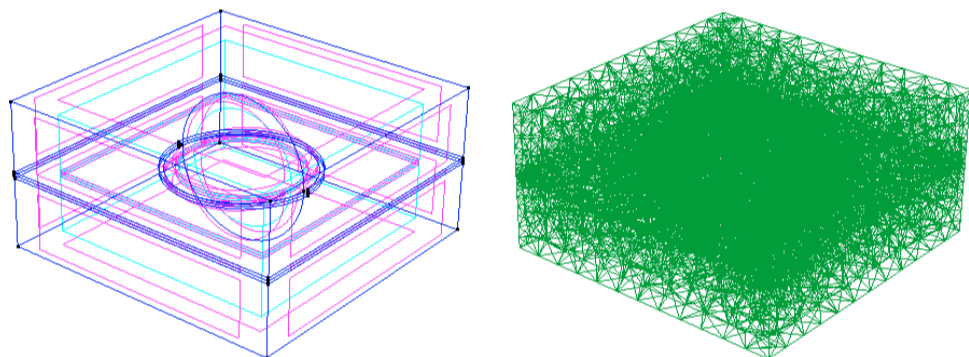
A visualisation package is provided

for the post processing of results. The director, order parameters, electric potential, velocity and pressure calculated by the model can be visualised over cut planes and iso-surfaces, which can be created, moved or deleted with ease. Incorporated in the package is an extended Jones optical code, which can be used to plot maps of the optical transmittance as well as viewing angle plots.

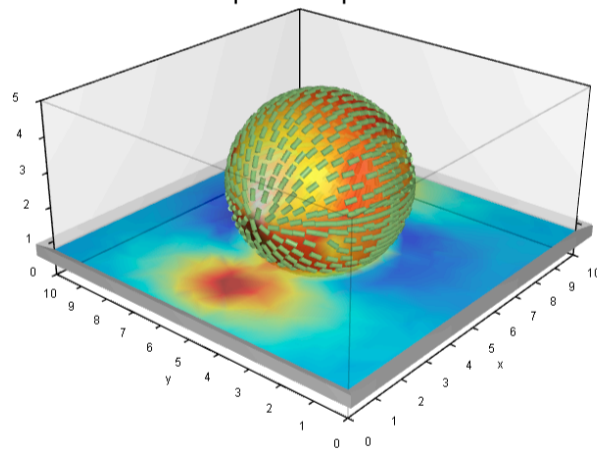
### Using the Program

The geometry of the liquid crystal device is entered using a CAD package. This allows complex shapes to be modelled, which may contain curved surfaces and protrusions into the liquid crystal layer.

The left hand figure below shows a liquid crystal cell containing a spherical spacer. Boundary conditions such as alignment surfaces and electrodes can be assigned. With the geometry defined the structure is then meshed by tetrahedral elements, as shown in the right hand figure.



Spherical Spacer

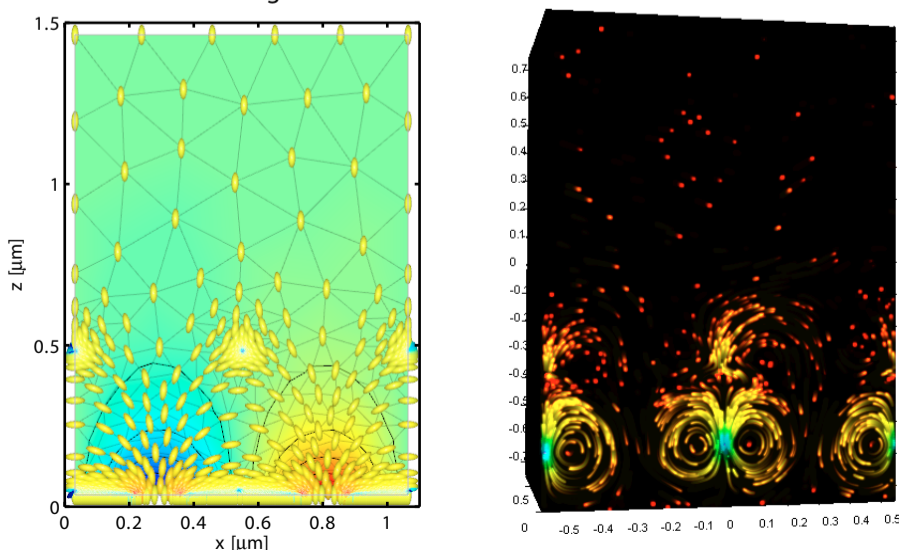


Material properties of the liquid crystal, such as elastic constants and viscosity coefficients, can then be defined as well as time varying voltages at the electrodes and the anchoring strength. Finally, the dynamic response of the liquid crystal is modelled.

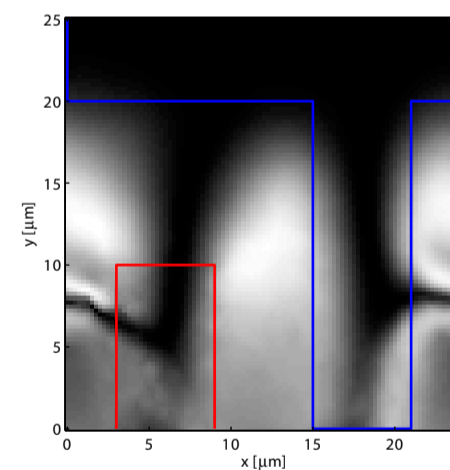
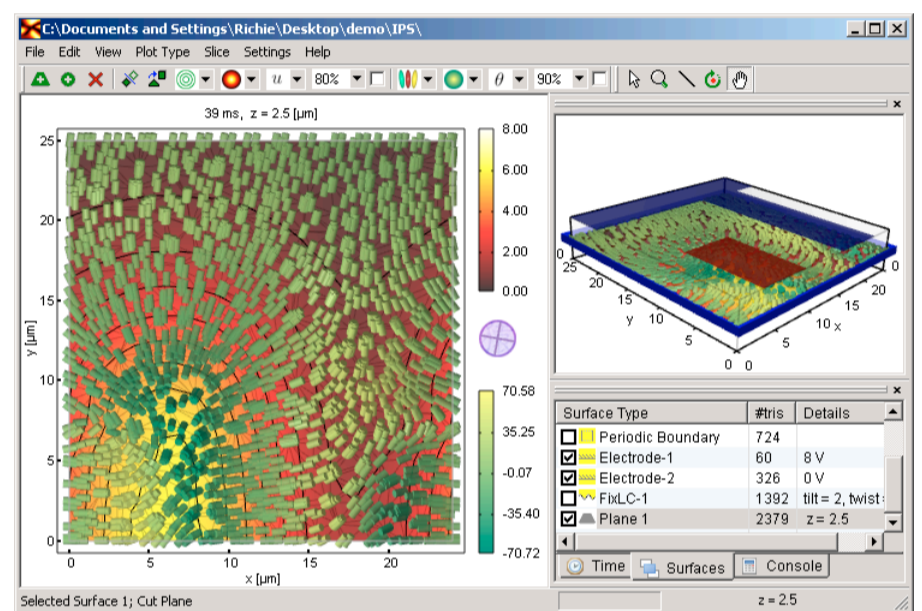
The figure to the left shows the simulation result, assuming that the anchoring over the surface of the sphere is planar degenerate.

### Defect Dynamics Including Flow

As devices become smaller, the high electric fields present in the shrinking inter-pixel gaps can give rise to defects within the liquid crystal. In the figure below defects are induced by a large electric field between interdigitated electrodes. The program is able to model accurately the movement of such defects, taking into account both the reorientation of the liquid crystal and its flow. For bistable devices these effects play a critical role in the switching between stable states.



### Visualisation - In Plane Switching Structure



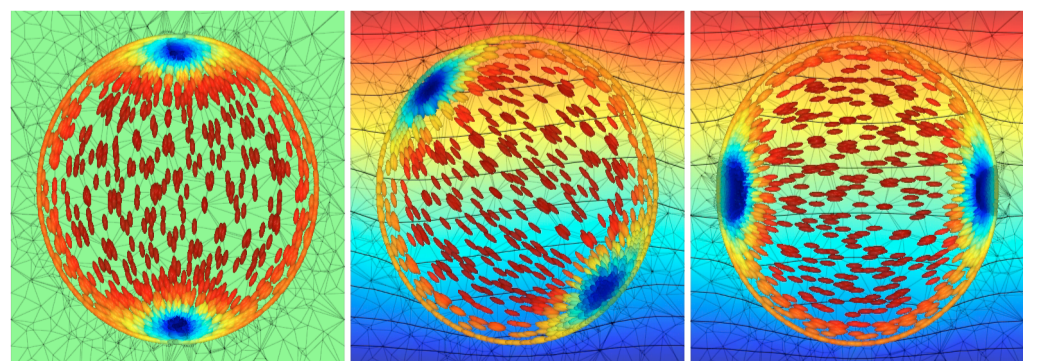
With the right hand pane of the visualiser cut planes may be created, moved and rotated.

The left hand pane shows the orthographic projection of this cut. Alternatively, this pane may be used to display surface or line plots.

A map of the optical transmittance, as shown in the figure to the left, is calculated using the extended Jones Method.

### Polymer Dispersed Liquid Crystal Droplets

A 3D simulation of a Polymer Dispersed Liquid Crystal (PDLC) droplet yields the results shown below. The director field and the electric potential (background colour) are shown on a cross-section through the structure.



### Other Capabilities

We have expertise in optical methods that take into account refraction and interference effects as well as diffraction. This includes the modelling of complete optical systems, through the combination of liquid crystal optical modelling techniques with the ray-tracing package ASAP. Other interests include waveguide modelling.