OpenLCDFDM: an finite-difference LCD simulator

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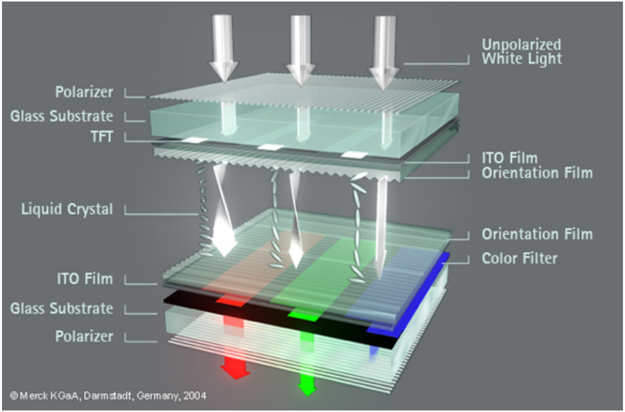
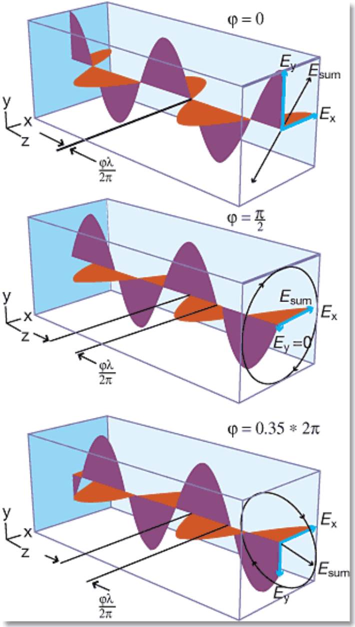
LCD on consumer products

LCD display structure

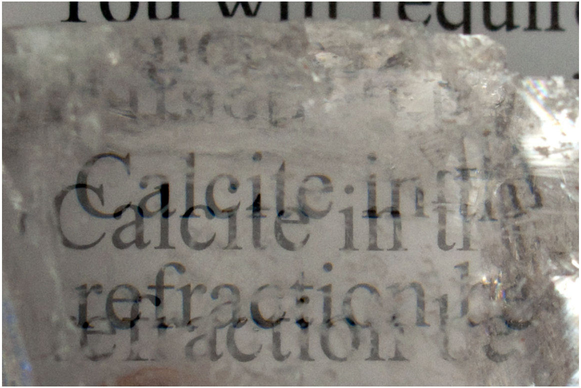


Liquid crystal layer is served as an optical switch, it determines how much light from light source (backlight in LCD display) can propagate through.

Polarization

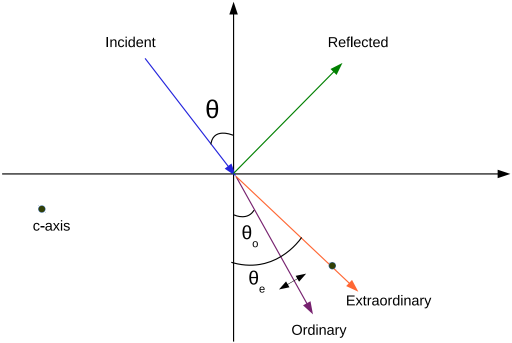


Birefringence



Birefringence

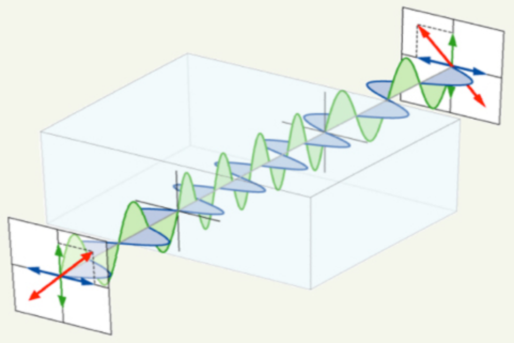
A material with two refractive index (n_o and n_e) means there are two refracted ray.



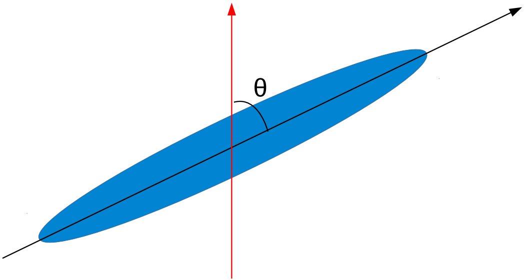
$$n_{air} \sin(\theta_1) = n_o \sin(\theta_o) \quad (1)$$
$$n_{air} \sin(\theta_1) = n_e \sin(\theta_e)$$

Birefringence

A material with two refractive index means that when light propagates through this material *it sees two light speed*.
The other important feature for birefringence is that it causes *phase retardation* and the polarization of light is changed.



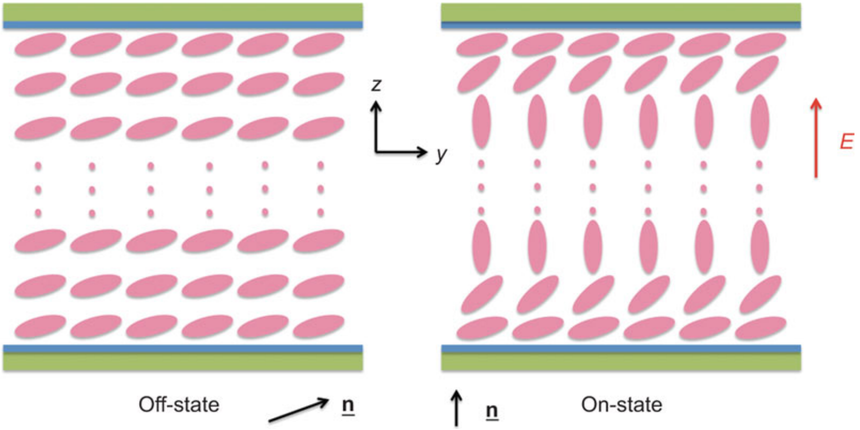
Birefringence



If the light incidents with an angle relative to the optical axis, the refractive index for extraordinary light is $n_e(\theta)$.

$$n_e(\theta) = \sqrt{\frac{\cos^2(\theta)}{{n_o}^2} + \frac{\sin^2(\theta)}{{n_e}^2}} \tag{2}$$

Electric controlled LC orientation



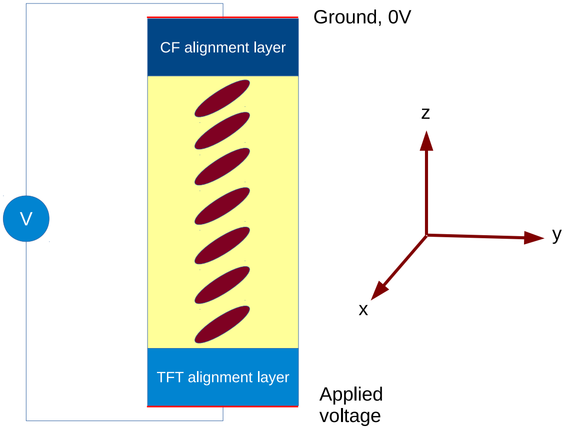
Due to the nonisotropic dielectric property of liquid crystal, when external electric field is applied, the LC molecule will start to align with the electric field.

Calculation models

In order to model such device, one has to model the transition liquid crystal orientation under electric field and calculate phase retardation under given LC distribution.

- Model LC distribution:
  - Oseen-frank free energy for liquid crystal
  - Laplace equation in nonisotropic media
- Optical calculation: Extended Jones matrix method

OpenLCDFDM 1D structure



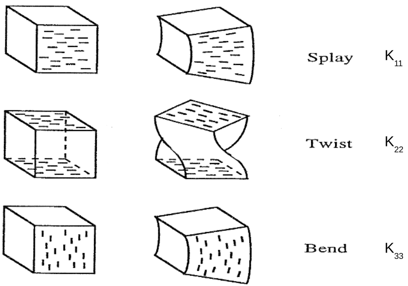
Calculate LC Orientation

Using Oseen-frank elastic free energy density to model the elastic property of the liquid crystal layer. The LC molecule distribution is acquired by minimizing the total energy density which includes elastic free energy density and electric field energy density. The total energy density has the following form [2].

$$\begin{aligned} f(\vec{x}) &= \frac{1}{2}K_{11}(\nabla \cdot \vec{n})^2 + \frac{1}{2}K_{22}(\vec{n} \cdot \nabla \times \vec{n})^2 + \frac{1}{2}K_{33}(\vec{n} \times \nabla \times \vec{n})^2 \\ &\quad + q_0 K_{22}(\vec{n} \cdot \nabla \times \vec{n}) - \frac{1}{2}(\vec{D} \cdot \vec{E}) \end{aligned}$$

where $\vec{D} = \overleftrightarrow{\epsilon}(\vec{x}) \cdot \vec{E}$ and $\overleftrightarrow{\epsilon}(\vec{x})$ is a 3X3 dielectric tensor. $\vec{n}(\vec{x})$ is a unit vector for local liquid crystal orientation.

Calculate LC Orientation



Calculate LC orientation

To calculate minimize free energy, *Euler-Lagrange equation* is applied. OpenLCDFDM uses finite difference method to solve Euler-Lagrange equation of the total energy density to get liquid crysal distribution of minimized free energy.
The Euler-Lagrange equation of the free energy is solved through iterative method.

$$\frac{\partial n_i}{\partial t} = \frac{1}{\gamma}\left(-\frac{\delta f}{\delta n_i}\right), i = x, y, z \tag{3}$$

γ is the rotational viscosity.

Laplace equation in nonisotropic and inhomogeneous media

Laplace equation:

$$\nabla \cdot \overleftrightarrow{\epsilon}(\vec{x}) \cdot \nabla \phi(\vec{x}) \quad = \quad 0$$

$\overleftrightarrow{\epsilon}(\vec{x})$ is the local dielectric tensor decided by the local oritation of LC molecule.

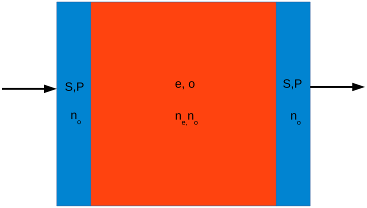
$$\overleftrightarrow{\epsilon}(\vec{x}) = \begin{bmatrix} \epsilon_\perp + \triangle\,\epsilon \sin^2\theta(\vec{x})\cos^2\phi(\vec{x}) & \frac{\triangle\epsilon}{2} sin^2\theta(\vec{x})\sin 2\phi(\vec{x}) & \frac{\triangle\epsilon}{2}\sin 2\theta(\vec{x})\cos\phi(\vec{x}) \\ \frac{\triangle\epsilon}{2}\sin^2\theta(\vec{x})\sin 2\phi(\vec{x}) & \epsilon_\perp + \triangle\,\epsilon \sin^2\theta(\vec{x})\sin^2\phi(\vec{x}) & \frac{\triangle\epsilon}{2}\sin 2\theta(\vec{x})\sin\phi(\vec{x}) \\ \frac{\triangle\epsilon}{2}\sin 2\theta(\vec{x})\cos\phi(\vec{x}) & \frac{\triangle\epsilon}{2}\sin 2\theta(\vec{x})\sin\phi(\vec{x}) & \epsilon_\perp + \triangle\,\epsilon\cos^2\theta(\vec{x}) \end{bmatrix}$$

where $\theta(\vec{x})$ and $\phi(\vec{x})$ is the local orientation of liquid crystal molecule, $\triangle\,\epsilon = \epsilon_{||} - \epsilon_\perp$.

Extended Jones matrix method for uniaixal media

Under the assumption of $n_e \approxeq n_o$, the e-ray and o-ray propagate on the same direction. With this assumption, Jones matrix can be modified into extended Jones matrix method.

$$\vec{J}_{out} = \begin{bmatrix} t'_s & 0 \\ 0 & t'_p \end{bmatrix} \begin{bmatrix} \vec{e}\cdot\vec{s} & \vec{o}\cdot\vec{s} \\ \vec{e}\cdot\vec{p} & \vec{o}\cdot\vec{p} \end{bmatrix} \begin{bmatrix} e^{ik_e \triangle z} & 0 \\ 0 & e^{ik_o \triangle z} \end{bmatrix} \begin{bmatrix} \vec{s}\cdot\vec{e} & \vec{p}\cdot\vec{e} \\ \vec{s}\cdot\vec{o} & \vec{p}\cdot\vec{o} \end{bmatrix} \begin{bmatrix} t_s & 0 \\ 0 & t_p \end{bmatrix} \vec{J}_{in}$$



t'_s, t'_p t'_s and t'_p are transmission rate for s wave and p wave acquired through Fresnel's euations.

Extended Jones matrix method for isotropic mediaand calculation for transmission rate

For isotropic media, the Jones matrix only needs to calculate transmission rate for s wave and p wave.

$$\vec{J}_{out} = \begin{bmatrix} t_s & 0 \\ 0 & t_p \end{bmatrix} \vec{J}_{in}$$

In above formulas, J_{in} and J_{out} are the Jones vectors of light.
Transmision rate for incoherent light source:

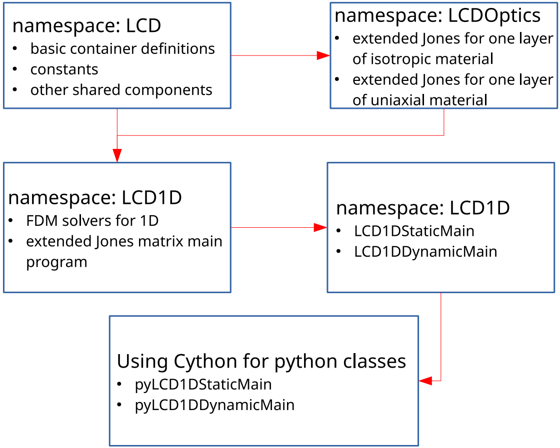
$$M = M_1 M_2 M_3 ... = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix}$$

$$T = 0.5 * (m_{11}^2 + m_{12}^2 + m_{21}^2 + m_{22}^2)$$

For multi-wavelength calculation:

$$T = \frac{\int T(\lambda) P(\lambda) V(\lambda) d\lambda}{\int P(\lambda) V(\lambda) d\lambda}$$

OpenLCDFDM program structures



Setup parameters for FDM solver

```
lcLayerNum = 40
lcThick = 4.0
lcCondition={'thick':lcThick, 'epsr_para':12.0, 'epsr_perp':3.6, 'gamma':60, \
    'k11':12.0, 'k22':6.5, 'k33':15.0, 'q0':2.0*np.pi/70.0}
rubbingCond={'tftTheta': 89.0*np.pi/180.0, 'tftPhi': 45.0*np.pi/180.0, 'cfTheta': \
    89.0*np.pi/180.0, 'totalTwist': 90.0*np.pi/180.0}
maxIter = 100000000
convergeError = 1.0e-8
lcd1dstaticmain = pyLCD1DStaticMain(lcLayerNum = lcLayerNum, dt = 0.01, \
    lcparam = lcCondition, rubbing = rubbingCond, voltStart = 0.0, voltEnd = 7.0, \
    voltStep = 0.1, maxIter = maxIter, convergeError = convergeError)
lcd1dstaticmain.setTFTPI(thick=0.1, epsr=3.6)
lcd1dstaticmain.setCFPI(thick=0.1, epsr=3.6)
```

Setup parameters for optical calculation

```
nk = readUniaxialSpectrum('TestPolarizerSpectrum.csv')
lcnk = readUniaxialSpectrum('TestLCSpectrum.csv')
pol_angle = [[90.0*np.pi/180.0, 135.0*np.pi/180.0]]
lcd1dstaticmain.addOpticalPolarizer(20.0, nk, pol_angle)
lcd1dstaticmain.addOpticalLC(lcThick, lcnk)
pol_angle = [[90.0*np.pi/180.0, 45.0*np.pi/180.0]]
lcd1dstaticmain.addOpticalPolarizer(20.0, nk, pol_angle)
lcd1dstaticmain.setOMPThreadNum(8)
lcd1dstaticmain.setOpticalIncidentAngles()
lcd1dstaticmain.setOpticalSourceSpectrum(readLightSourceSpectrum('TestLightSrc.csv'))
lcd1dstaticmain.setOpticalWavelength(0.38, 0.78, 0.01)
lcd1dstaticmain.useOptical2X2Lambertian()
lcd1dstaticmain.createExtendedJones()
```

Calculate and get results

```
lcd1dstaticmain.calculate()
transmissions = np.array(lcd1dstaticmain.getTransmissions())
directors = np.array(lcd1dstaticmain.getLCDirResults())
inAngles = np.array(lcd1dstaticmain.getIncidentAngles())
calcVolts = np.array(lcd1dstaticmain.getCalcVolts())
normalTrans = np.array(lcd1dstaticmain.getNormalTransmissions())
```

Demo: V-T curve of TN mode

Future works

- Calculate Stokes values to track change of polarization.
- Implement Berreman 4X4 method
- Add bixial material support for extended Jones matrix method
- Bind OpenLCDFDM with FDTD simulation module(ex. meep-FDTD)
- Move toward 2D and 3D simulation

References

- Optics of Liquid Crystal Display by Pochi Yeh and Claire Gu. ISBN: 0470181761
- Fundamentals of Liquid Crystal Devices by Shin-Tson Wu and Deng-Ke Yang. ISBN: 978-0-470-03202-2