How to calculate the LC director field

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Introduction to LC modeling methods

- LC configurations in the equilibrium state
  ⇔ calculation of the minimum free energy
  (Gibb's free energy)

- **Gibb's free energy = elastic energy + electric energy**
  ⇔ $\mathbf{F_g = F_s + F_e}$

$$F_g = \int_v f_g \, dv \quad \rightarrow \quad f_g : Gibb's \ free \ energy \ density$$

- Calculation for the equilibrium state (Minimum energy state)

  1) Euler-Lagrange equations

$$0 = -[f_g]_n$$

$$0 = -[f_g]_V = \nabla \cdot D = \nabla \cdot (\varepsilon_0 \varepsilon_r \nabla V)$$

$[f_g]_n$: *Functional Delivatives by* n

$[f_g]_V$: *Functional Delivatives by voltage* V

2) Dynamic equation and relaxation method

$$\gamma_1 \frac{\Delta n}{\Delta t} = -[f_g]_n \quad : Discretized\ form$$

$$\Rightarrow \Delta n = -\frac{\Delta t}{\gamma_1}([f_g]_n)$$

So, $\overline{n}^{\tau+1} = n^{\tau} - \frac{\Delta t}{\gamma_1}[f_g]_n$: Calculation of new director

3) Normalization $\Leftrightarrow$ Unitization of the director

- Oseen-Frank Equation's Vevtor form

- In general, deformation of LC directors (Elastic term) can be achieved from *Oseen-Frank* equation (*Vector form*)

$$fs = \frac{1}{2} K_{11} (\nabla \cdot n)^2 + \frac{1}{2} K_{22} (n \cdot \nabla \times n)^2 + \frac{1}{2} K_{33} (n \times \nabla \times n)^2$$

- Electric free energy

$$fe = \frac{1}{2} E \varepsilon_o \bar{\varepsilon} E \quad E = -\nabla V$$

- *Euler-Lagrange* equations for vector method

$$0 = -[f_g]_{n_i}$$

$$0 = -[f_g]_V = \nabla \cdot D = \nabla \cdot (\varepsilon_0 \varepsilon_r \nabla V)$$

$$[f_g]_{n_i} : Functional\ \ Delivatives\ \ by\ n_i$$

$$[f_g]_V : Functional\ \ Delivatives\ \ by\ voltage V$$

$$[f_g]_{n_i} = \frac{\partial f_g}{\partial n_i} - \frac{d}{dx}\left(\frac{\partial f_g}{\partial n_{i,x}}\right) - \frac{d}{dx}\left(\frac{\partial f_g}{\partial n_{i,y}}\right) - \frac{d}{dx}\left(\frac{\partial f_g}{\partial n_{i,z}}\right)$$

$$n_{i,x} = \frac{\partial n_i}{\partial x}, \quad n_{i,y} = \frac{\partial n_i}{\partial y}, \quad n_{i,z} = \frac{\partial n_i}{\partial z}$$

- Dynamic equation and relaxation method for Vector method

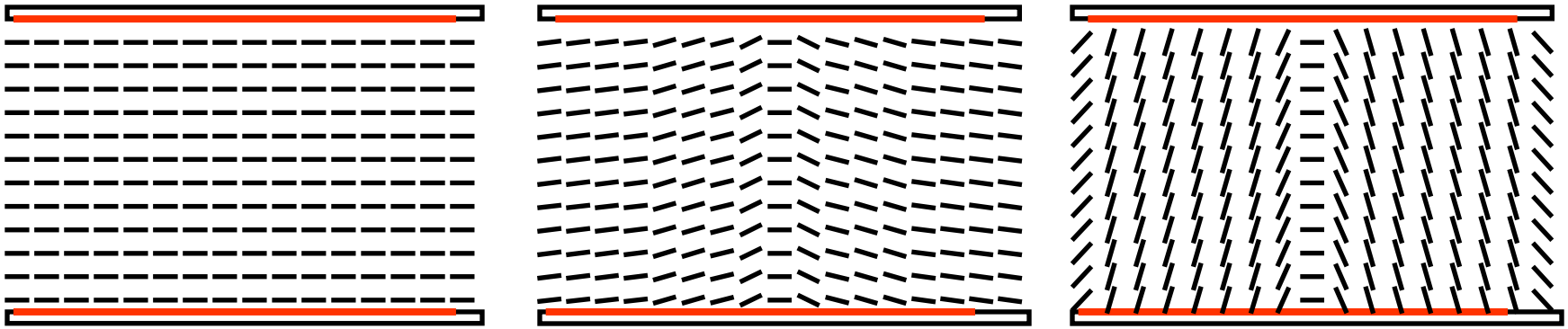
$$\gamma_1 \frac{\Delta n_i}{\Delta t} = -[f_g]_{n_i} \quad : Discretized\ form \qquad \Rightarrow \Delta n_i = -\frac{\Delta t}{\gamma_1}([f_g]_{n_i})$$

Therefore $$\overset{-\tau+1}{n}_i = n_i^{\tau} - \frac{\Delta t}{\gamma_1}[f_g]_{n_i}$$

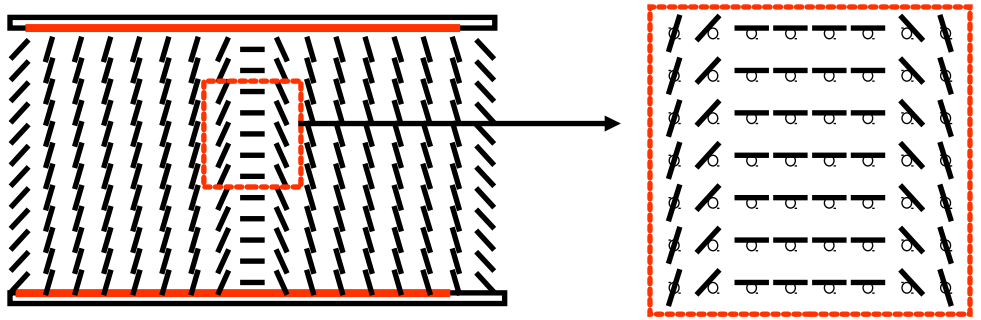
- Normalization $$n_i^{\tau+1} = \frac{\overset{-\tau+1}{n}_i}{\left|\overset{-\tau+1}{n}_i\right|}$$

- Discussion

– Vector notation but actual directors is not vector properties
– Simple calculation
– Different energies between (*n*, *n*) and (*n*, -*n*), so that this is a non physical and does not allow transitions between topological aninequivalence , for example, in the case of a pixel with increasing voltage

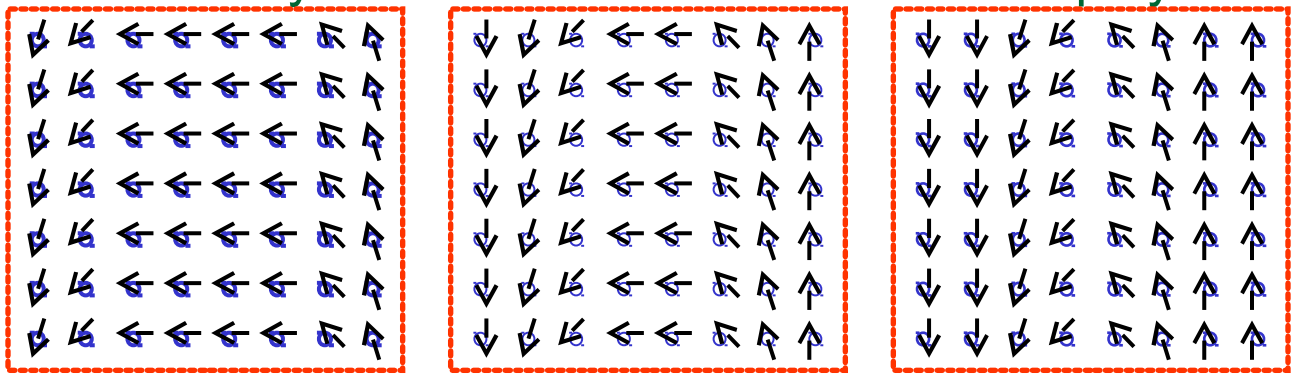


Now look at only the small region in the middle of the pixel, and consider the grid points used in the simulation



As further increase voltage, eventually the horizontal region will fall between the grid points. But the bend distortion cannot be removed.

There is no way to have the transition from the splay to bend state



– Can't calculate order parameter *S*, so that this can't model the defects

- **Flow chart for calculation (Vector method)(LC3D by James Anderson)**