A finite element method for the Ericksen model with colloidal effects and external fields

Shawn W. Walker

Louisiana State University
Department of Mathematics and
Center for Computation and Technology (CCT)

Supported by the National Science Foundation
DMS-1418994, DMS-1555222 (CAREER)
Numerical analysis:
- Ricardo H. Nochetto, University of Maryland, Mathematics
- Wujun Zhang, Rutgers, Mathematics

Modeling with colloids:
- Maria-Carme Calderer, University of Minnesota, Mathematics
- Dmitry Golovaty, University of Akron, Mathematics

Phase-field methods:
- Amanda Diegel (postdoc), Louisiana State University, Mathematics
# Table of Contents

1. Introduction
2. Discrete Energy and FEM
3. Gradient Flow
4. Simulations
5. Colloids
6. Immersed Boundary
7. Electric Field
8. Cahn-Hilliard
9. Conclusion
What Are Liquid Crystals?

- Liquid crystal (LC) *molecules* look like elongated rods.
What Are Liquid Crystals?

- Liquid crystal (LC) *molecules* look like elongated rods.

- Liquid crystals (LCs) can manipulate light (and do other cool stuff).
Order parameters \( \mathbf{n} \) and \( s \) come from averaging over LC molecules:

- **Unit vector** \( \mathbf{n} \)
  - represents average orientation.

\[ n = \frac{3 \cos^2 \theta - 1}{2} \]

\[ -\frac{1}{2} \leq s \leq 1 \]

\( n \theta \) well-aligned

Equilibrium states of LCs are energy minimizers.

Different models: Oseen-Frank, Ericksen, \( Q \)-tensor.

FEM for the Ericksen Model

S. W. Walker
Order parameters $n$ and $s$ come from averaging over LC molecules:

- **Unit vector $n$** represents average orientation.
- **Scalar $s$** represents the *degree of orientation*:
  \[
  s = \left\langle \frac{3 \cos^2 \theta - 1}{2} \right\rangle \Rightarrow -1/2 \leq s \leq 1.
  \]
  
  $s \gg 0$ well-aligned
  
  $s \approx 0$ local defect

- Equilibrium states of LCs are energy minimizers.
- Different models: Oseen-Frank, **Ericksen**, $Q$-tensor.
Ericksen’s Model

- The equilibrium state minimizes (one-constant Ericksen’s model):

\[
E[s, n] := \int_{\Omega} \kappa |\nabla s|^2 + s^2 |\nabla n|^2 \, dx + \int_{\Omega} \psi_B(s) \, dx
\]

\[=: E_1 + E_2\]

where \(\kappa > 0\) and \(\psi_B\) is a double well potential.

- \(s\) is the **degree of orientation** \((-1/2 \leq s \leq 1)\).
- \(s = 1\): perfect alignment with \(n\).
- \(s = 0\): no preferred direction (isotropic). This defines the set of defects:

\[
\{x \in \Omega, \ s(x) = 0\}.
\]

- \(s = -1/2\): perpendicular to \(n\).

The Ericksen model regularizes defects.
Literature Review

Ambrosio (1990)
Ball Zarnescu (2011)

Alouges (1997)
Bartels (2010)
Cohen Lin Luskin (1989)
Liu Walkington (2000)
Yang Forest Li Liu Shen Wang (2013)

Barrett Feng Prohl (2006) (2D-FEM via regularization)
James Willman Fernández (2006) (Q tensor method)
Shin Cho Lee Yoon and Won (2008) (Q tensor method)
Structure of the Energy

\[ E_1[s, n] := \int_{\Omega} \kappa |\nabla s|^2 + s^2 |\nabla n|^2 \, dx. \]

- The constraint \(|n| = 1\) implies \(\nabla |n|^2 = 2n^T (\nabla n) = 0\), which yields an identity:

\[
\int_{\Omega} |\nabla (sn)|^2 \, dx = \int_{\Omega} |n \otimes \nabla s + s \nabla n|^2 \, dx = \int_{\Omega} |\nabla s|^2 + s^2 |\nabla n|^2 \, dx.
\]
Structure of the Energy

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\int_{\Omega} |\nabla (sn)|^2 \, dx = \int_{\Omega} |n \otimes \nabla s + s \nabla n|^2 \, dx = \int_{\Omega} |\nabla s|^2 + s^2 |\nabla n|^2 \, dx =: u.
\]

- Thus, we rewrite the energy [Ambrosio 90, Lin 91]:

\[ E_1[s, n] = E_1[s, u] = \int_{\Omega} (\kappa - 1)|\nabla s|^2 + |\nabla u|^2 \, dx, \]

i.e. a quadratic functional with a negative term.

- This implies the following admissible class:

\[ A := \{(s, n) : s \in H^1(\Omega), \ u = sn \in H^1(\Omega) \text{ and } |n| = 1 \text{ a.e. in } \Omega \}. \]
Discretization Framework

- Piecewise linear approximations: \( s_h \) in \( S_h \), \( n_h \) in \( N_h \):

\[
S_h := \{ s_h \in H^1(\Omega) : s_h|_T \text{ is affine} \},
\]

\[
U_h := \{ u_h \in H^1(\Omega)^d : u_h|_T \text{ is affine in each component} \},
\]

\[
N_h := \{ n_h \in U_h : |n_h(x_i)| = 1 \text{ at all nodes } x_i \in N_h \},
\]

defined over a conforming, shape-regular triangulation (mesh) of \( \Omega \).
Discretization Framework

- Piecewise linear approximations: $s_h$ in $S_h$, $n_h$ in $N_h$:
  
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  $$

defined over a conforming, shape-regular triangulation (mesh) of $\Omega$.

- $\{\phi_i\}$ are continuous piecewise linear “hat” basis functions.

- Assume the entries of the stiffness matrix $\{k_{ij}\}$ satisfy

  $$
  k_{ij} := -\int_{\Omega} \nabla \phi_i \cdot \nabla \phi_j \, dx \geq 0, \quad \text{for } i \neq j.
  $$

- If the mesh is weakly acute (or non-obtuse), then this condition is true.
Need a *discrete version* of:

\[ E_1[s, n] = \int_\Omega (\kappa - 1)|\nabla s|^2 + |\nabla u|^2 dx, \quad \text{with } u = sn. \]

Since \( |n_h(x)| = 1 \) only at the nodes \( x = x_i \), write the discrete energy in terms of **nodal values**.
Discretization of the Energy

• Need a *discrete version* of:

\[
E_1[s, n] = \int_{\Omega} (\kappa - 1)|\nabla s|^2 + |\nabla u|^2 \, dx, \quad \text{with } u = sn.
\]

• Since \(|n_h(x)| = 1\) *only at the nodes* \(x = x_i\), write the discrete energy in terms of nodal values.

• We approximate \(E_1\) by \(E_1^h\):

\[
E_1 = \kappa \int_{\Omega} |\nabla s|^2 \, dx + \int_{\Omega} s^2 |\nabla n|^2 \, dx,
\]

\[
E_1^h := \frac{\kappa}{2} \sum_{i,j=1}^{N} k_{ij} (s_i - s_j)^2 + \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left( \frac{s_i^2 + s_j^2}{2} \right) |n_i - n_j|^2,
\]

where \(n_i = n_h(x_i)\).
Stability of the Discrete Energy

- Let $u_h$ in $U_h$ such that $u_h(x_i) = s_h(x_i)n_h(x_i)$ for all nodes $x_i$.

Discrete identity:

$$E_h^1[s_h, n_h] = (\kappa - 1) \int_\Omega |\nabla s_h|^2 dx + \int_\Omega |\nabla u_h|^2 dx + E$$

$$\geq (\kappa - 1) \int_\Omega |\nabla s_h|^2 dx + \int_\Omega |\nabla u_h|^2 dx,$$

where

$$E := \sum_{i,j=1}^{N} k_{ij} (s_i - s_j)^2 \left| \frac{n_i - n_j}{2} \right|^2 \geq 0.$$
Stability of the Discrete Energy

- Let \( u_h \) in \( \mathbb{U}_h \) such that \( u_h(x_i) = s_h(x_i)n_h(x_i) \) for all nodes \( x_i \).

- Discrete identity:

\[
E_h^{1}[s_h, n_h] = (\kappa - 1) \int_{\Omega} |\nabla s_h|^2 dx + \int_{\Omega} |\nabla u_h|^2 dx + \mathcal{E} \\
\geq (\kappa - 1) \int_{\Omega} |\nabla s_h|^2 dx + \int_{\Omega} |\nabla u_h|^2 dx,
\]

where

\[
\mathcal{E} := \sum_{i,j=1}^{N} k_{ij} (s_i - s_j)^2 \left| \frac{n_i - n_j}{2} \right|^2 \geq 0.
\]

- Along with several other technical results, we are able to show \( \Gamma \)-convergence of minimizers.

- Nochetto, W., Zhang, in review at SINUM.

- Music video summary: see my web-site or you-tube:

  - https://www.youtube.com/watch?v=pWWw7_6cQ-U
We want to show there exists a sequence such that
\[ E_1[s, u] = \lim_{h \to 0} E_1^h[s_h, u_h] \]

- Regularize: \((\hat{s}, \hat{u})\) and define \(s_h = I_h \hat{s}, \ u_h = I_h \hat{u}\).
- The regularization \((\hat{s}, \hat{u})\) needs to be in the admissible set \(A(g, r)\), i.e.
  \[ |\hat{s}| = |\hat{u}| \]
- Moreover, \((s_h, u_h)\) needs to be in \(A_h(g_h, r_h)\), i.e.
  \[ |s_h(x_i)| = |u_h(x_i)|, \quad \text{at all nodes.} \]
We want to show there exists a sequence such that

\[ E_1[s, u] = \lim_{h \to 0} E_1^h[s_h, u_h] \]

**Regularize:** \((\hat{s}, \hat{u})\) and define \(s_h = I_h \hat{s}, u_h = I_h \hat{u}\).

The regularization \((\hat{s}, \hat{u})\) needs to be in the admissible set \(A(g, r)\), i.e.

\[ |\hat{s}| = |\hat{u}| \]

Moreover, \((s_h, u_h)\) needs to be in \(A_h(g_h, r_h)\), i.e.

\[ |s_h(x_i)| = |u_h(x_i)|, \quad \text{at all nodes.} \]

**Construction:**

\[ s_\delta := d_\delta (s \ast \eta_\delta) + (1 - d_\delta)g, \quad u_\delta := d_\delta (u \ast \eta_\delta) + (1 - d_\delta)r, \]

and the define

\[ \hat{s} = s_{\sigma, \delta} := \rho_{\sigma}(s_\delta)|u_\delta|, \quad \hat{u} = u_{\sigma, \delta} := |\rho_{\sigma}(s_\delta)|u_\delta, \]

where \(\rho_{\sigma}(t)\) is a Lipschitz approximation of the “sign” function.
Alternating Direction Method

- Alternate minimizing $E^h[s_h, n_h]$ with respect to $s_h$ and $n_h$. 
Alternating Direction Method

- Alternate minimizing $E^h[s_h, n_h]$ with respect to $s_h$ and $n_h$.
- Introduce the **discrete tangent space** [Alouges 97, Bartels 10] at the $k$-th iteration:

$$T^k_h = \{ t_h \in H^1(\Omega), \; t_h|_T \text{ is affine, and } t_i \cdot n^k_i = 0 \; \text{for all nodes } x_i \}.$$
Alternating Direction Method

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For $k = 0, 1, 2, ...$

1. **Step (a):** minimize in the tangent space:

   $$\text{find } t^k_h \in T^k_h : \quad E^1_h[s^k_h,n^k_h + t^k_h] \leq E^1_h[s^k_h,n^k_h + v_h], \quad \forall v_h \in T^k_h,$$

   i.e. find $t^k_h \in T^k_h : \quad \delta_n E^1_h[s^k_h,n^k_h + t^k_h, v_h] = 0, \quad \forall v_h \in T^k_h.$
Alternating Direction Method

- Alternate minimizing $E^h[s_h, n_h]$ with respect to $s_h$ and $n_h$.
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For $k = 0, 1, 2, ...$

- **Step (a):** minimize in the tangent space:

  $$\text{find } t^k_h \in T^k_h : \ E_1^h[s^k_h, n^k_h + t^k_h] \leq E_1^h[s^k_h, n^k_h + v_h], \quad \forall v_h \in T^k_h,$$

  i.e. find $t^k_h \in T^k_h : \ \delta_{n_h} E_1^h[s^k_h, n^k_h + t^k_h, v_h] = 0, \quad \forall v_h \in T^k_h$.

- **Step (b):** project: $n^k_{i+1} := \frac{n^k_i + t^k_i}{|n^k_i + t^k_i|}$, at all nodes.
Alternating Direction Method

- Alternate minimizing $E^h[s^k_h, n^k_h]$ with respect to $s^k_h$ and $n^k_h$.
- Introduce the **discrete tangent space** [Alouges 97, Bartels 10] at the $k$-th iteration:

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For $k = 0, 1, 2, ...$

- **Step (a):** minimize in the tangent space:

  $$\text{find } t^k_h \in T^k_h : \ E^h_1[s^k_h, n^k_h + t^k_h] \leq E^h_1[s^k_h, n^k_h + v_h], \ \forall v_h \in T^k_h,$$

  i.e. find $t^k_h \in T^k_h : \ \delta_{n^k_h} E^h_1[s^k_h, n^k_h + t^k_h, v_h] = 0, \ \forall v_h \in T^k_h$.

- **Step (b):** project: $n^k+1_i := \frac{n^k_i + t^k_i}{|n^k_i + t^k_i|}$, at all nodes.

- **Step (c):** $L^2(\Omega)$-gradient flow: find $s^{k+1}_h$ in $S_h$ such that:

$$\int_\Omega \frac{s^{k+1}_h - s^k_h}{\delta t} z_h = -\delta_{s^k_h} E^h_1[s^{k+1}_h, n^{k+1}_h; z_h] - \delta_{s^k_h} E^h_2[s^{k+1}_h; z_h], \ \forall z_h \in S_h.$$

Delivers a monotone energy decreasing scheme.
Plane Defect in 3-D [Ambrosio, Virga 1991]

- \( \mathbf{n} = \mathbf{e}_1 \) on \( S^- \), \( \mathbf{n} = \mathbf{e}_2 \) on \( S^+ \). Set \( s = s^* \) on \( S^+ \) and \( S^- \).
- \( \kappa := 0.2 \) yields a set of defect: \( \{ z = 1/2 \} \).

\[
\| s - s_h \|_{L^2(\Omega)} \quad O(h) \\
\| s - s_h \|_{H^1(\Omega)} \quad O(h^{1/2}) \\
\| \mathbf{n} - \mathbf{n}_h \|_{L^2(\Omega)} \quad O(h^{1/2}) \\
\| \mathbf{u} - \mathbf{u}_h \|_{L^2(\Omega)} \quad O(h) \\
\| \mathbf{u} - \mathbf{u}_h \|_{H^1(\Omega)} \quad O(h^{1/2})
\]
“X” Defect in 3-D \((\kappa = 0.1)\)

MOovie: Director Evolution
“X” Defect in 3-D ($\kappa = 0.1$)

Colloidal dispersions provide an avenue toward new micro- and nano-functional materials.

Simple colloid/particle shapes can induce a variety of ordered and disordered structures.

Basic mechanism: self-assembly through energy minimization.

Varying surface treatment, e.g. Janus particles, etc.

Defects Near Inclusions

- Spherical inclusion.
- Planar anchoring on outer boundary.
- Normal anchoring on sphere.
- Saturn ring defect.
- $\mathbf{Q}$-tensor used in the modeling.

Illustration of line field.

- Figure taken from Alama, Bronsard, Lamy, PRE, vol. 93, 2016.
Non-obtuse 3-D Mesh with Inclusion

- Not easy to generate **non-obtuse** meshes of complex domains.
- Open problem whether this can be done in general.
Non-obtuse 3-D Mesh with Inclusion

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- Open problem whether this can be done in general.

Our example:
- Create a prism of ideal (well-centered) tetrahedra.
- Remove a spherical hole of the “right size.”
- Perform two well-chosen refinements (with mild deformations of the mesh).
- Resulting mesh is non-obtuse, i.e. all dihedral angles are $\leq 90^\circ$.

Computational mesh.
DEFECTS NEAR INCLUSIONS: 1ST BOUNDARY CONDITION

- **Non-obtuse** mesh with spherical inclusion.
- Planar anchoring on outer boundary.
- Normal anchoring on sphere.
- Disperse Defect Vs. Point Defect.
- MOVIE: $\kappa = 0.1$ MOVIE: $\kappa = 1.0$

Conclusion
Defects Near Inclusions: 2nd Boundary Condition

- Non-obtuse mesh with spherical inclusion.
- **Smoothed** anchoring on outer boundary.
- Normal anchoring on sphere.
- Ring-like Defect.
- MOVIE: $\kappa = 1.0$

Computational mesh.
We want to preserve the non-obtuse mesh property with variable domain.

Use a level set representation of the reference colloid domain $\hat{\Omega}_c$.

Let $\hat{d} : \mathbb{R}^n \to \mathbb{R}$ be a level set function, whose zero level set corresponds to $\partial \hat{\Omega}_c$. 
We want to preserve the non-obtuse mesh property with variable domain.

Use a level set representation of the reference colloid domain $\hat{\Omega}_c$.

Let $\hat{d} : \mathbb{R}^n \to \mathbb{R}$ be a level set function, whose zero level set corresponds to $\partial \hat{\Omega}_c$.

Actual colloid $\Omega_c$ is obtained by a rigid motion, i.e. $\hat{\Omega}_c = F(\Omega_c)$ defined by

$$\hat{x} = F(x) = Rx + b.$$
Phase-Field Representation of Colloids

- Define a 1-D phase-field function $\phi_{\text{ref}} : (-\infty, \infty) \rightarrow (0, 1)$:

$$
\phi_{\text{ref}}(t) = \frac{1}{2} \left[ \frac{2}{\pi} \arctan \left( -\frac{t}{\epsilon} \right) + 1 \right],
$$

where $\epsilon > 0$ is the thickness of the transition.

- Represent colloid by a phase-field function:

$$
\phi(x) = \phi_{\text{ref}}(d(x)) = \phi_{\text{ref}}(\hat{d}(F(x))).
$$
Phase-Field Representation of Colloids

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  where $\epsilon > 0$ is the thickness of the transition.
- Represent colloid by a phase-field function:
  $$\phi(x) = \phi_{\text{ref}}(d(x)) = \phi_{\text{ref}}(\hat{d}(F(x))).$$

- Immersed boundary method.
- Gives a regularized approximation of perimeter:
  $$C_0 \frac{\epsilon}{2} \int_{\Omega} |\nabla \phi(x)|^2 dx \to |\partial \Omega_c|,$$
  as $\epsilon \to 0$. 

\[\text{FEM for the Ericksen Model}\]
Weak Anchoring

- We treat the surface of the colloid as a rigid shell, with liquid crystal material contained *inside and outside* (for simplicity).
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- Oseen-Frank (normal anchoring):

  \[
  \frac{K_a}{2} C_0 \epsilon \int_{\Omega} |n|^2 |\nabla \phi|^2 - (\nabla \phi \cdot n)^2 \, dx.
  \]

- \(Q\)-tensor:

  \[
  \frac{K_a}{2} C_0 \epsilon \int_{\Omega} |\nabla \phi|^2 |Q - Q^*|^2 \, dx.
  \]
Weak Anchoring

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- Oseen-Frank (normal anchoring):

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\]

- Q-tensor:

\[
\frac{K_a}{2} C_0 \epsilon \int_{\Omega} |\nabla \phi|^2 |Q - Q^*|^2 \, dx.
\]

- Ericksen (normal anchoring):

\[
E_a[s, n, \phi] = \frac{K_a}{2} C_0 \epsilon \int_{\Omega} s^2 \left[ |n|^2 |\nabla \phi|^2 - (\nabla \phi \cdot n)^2 \right] \, dx \\
+ \frac{K_a}{2} C_0 \epsilon \int_{\Omega} |\nabla \phi|^2 (s(x) - s^*)^2 \, dx.
\]
Weak Anchoring Discretization

- **Mass lumping:**

\[ E_a^h[s_h, n_h, \phi] = \frac{K_a}{2} C_0 \epsilon \int_{\Omega} I_h \left\{ s_h^2 \left[ |n_h|^2 |\nabla \phi|^2 - (\nabla \phi \cdot n_h)^2 \right] \right\} dx \]

\[ + \frac{K_a}{2} C_0 \epsilon \int_{\Omega} |I_h \nabla \phi|^2 (s_h(x) - s^*)^2 dx, \]

where \( I_h \) is the Lagrange interpolant.

- \( \Gamma \)-convergence is (essentially) the same as before.
Revisit Saturn Ring

1st B.C.:

2nd B.C.:
While minimizing $E$ with respect to $s_h$ and $n_h$, we optimize the colloid’s configuration.

Finite dimensional optimization for the rigid motion:

$$F(x) = R(\theta, r)x + b.$$ 

Control Parameters: $b$, $\theta$, and $r$.

Simulation: Disk 2-D
Simulation: Ellipse 2-D
Simulation: Two Disks (A)
Simulation: Two Disks (B)
Simulation: Sphere 3-D
Recall the energy:

- $E_1[s, \mathbf{n}] = \int_{\Omega} \left( \kappa |\nabla s|^2 + s^2 |\nabla \mathbf{n}|^2 \right) dx.$
- $E_2[s, \mathbf{n}] = \int_{\Omega} \psi(s) dx.$

Following de Gennes, Prost, 1995 and Biscari, Cesana, 2007, we have:

- $E[s, \mathbf{n}] = E_1[s, \mathbf{n}] + E_2[s] + E_{ext}[s, \mathbf{n}]$, where

  $$E_{ext}[s, \mathbf{n}] = -\frac{K_{ext}}{2} \left( \bar{\varepsilon} \int_{\Omega} (1 - s \gamma_a) |\mathbf{E}|^2 + \varepsilon_a \int_{\Omega} s (\mathbf{E} \cdot \mathbf{n})^2 \right).$$

- Reflects the anisotropic nature of the material.
- All constants are positive.
- Adds a lower order, bounded **negative** term to the energy.
The electrical energy is approximated by a \textit{mass-lumped} version of

\[
E^h_{\text{ext}}[s_h, n_h] = \frac{K_{\text{ext}}}{2} \left( -\bar{\varepsilon} \int_\Omega (1 - s_h \gamma_a) |\mathbf{E}|^2 - \varepsilon_a \int_\Omega s_h (\mathbf{E} \cdot n_h)^2 
+ |\varepsilon_a| \int_\Omega |\mathbf{E}|^2 (|n_h|^2 - 1) \right).
\]

- “Extra” term is non-positive and \textit{consistent} (i.e. it vanishes as \(h \rightarrow 0\)).
- \(\int_\Omega |\mathbf{E}|^2 |n|^2\) is constant at the continuous level.
- Does not fundamentally change the energy.
- It is needed to ensure the projection step in the algorithm decreases the (discrete) energy.
The Freedericksz Transition

[Brochard, 1975], [Virga, 1994], [deGennes, Prost, 1995],
[Biscari, Cesana, 2007]

Figure from: Hoogboom, Elemans, Rowan, Rasing, Nolte,

MOVIE
Electric Field and Saturn Ring

Parameters:
- Same boundary conditions as the Saturn ring case.
- \( \kappa = 1.0 \)
- \( K_{\text{ext}} = 160, \bar{\varepsilon} = 1.0, \varepsilon_a = 2.0, \gamma_a = 0.5, \quad \mathbf{E} = (0, 1, 0) \)
- Iso-surface shown: \( s = 0.08 \).
Moving Colloids With Electric Fields


- Simulation: Optimize a “sausage” shape
- Include an electric field: $K_{\text{ext}} = 80$, $\bar{\epsilon} = 1.0$, $\epsilon_a = 2.0$, $\gamma_a = 0.5$, $\mathbf{E} = (1, 0)$.

Simulation: Electric Field
Liquid crystal droplets: find equilibrium shapes via Cahn-Hilliard flow coupled to Ericksen.

Energy functional: \((s, n) \in \mathbb{A}(g, r)\) and \(\phi \in H^1(\Omega)\):

\[
E[s, n, \phi] = E_1[s, n] + E_2[s] + \frac{1}{4\varepsilon} \int_\Omega (\phi^2 - 1)^2 + \frac{\varepsilon}{2} \int_\Omega |\nabla \phi|^2 \\
+ \frac{\varepsilon}{2} \int_\Omega s^2 \left[|n|^2|\nabla \phi|^2 - (n \cdot \nabla \phi)^2\right] + \frac{\varepsilon}{2} \int_\Omega |\nabla \phi|^2 (s - s^*)^2.
\]
Liquid crystal droplets: find equilibrium shapes via Cahn-Hilliard flow coupled to Ericksen.

Energy functional: \((s, n) \in A(g, r)\) and \(\phi \in H^1(\Omega)\):

\[
E[s, n, \phi] = E_1[s, n] + E_2[s] + \frac{1}{4\varepsilon} \int_\Omega (\phi^2 - 1)^2 + \frac{\varepsilon}{2} \int_\Omega |\nabla \phi|^2 \\
+ \frac{\varepsilon}{2} \int_\Omega s^2 \left[|n|^2|\nabla \phi|^2 - (n \cdot \nabla \phi)^2\right] + \frac{\varepsilon}{2} \int_\Omega |\nabla \phi|^2 (s - s^*)^2.
\]

Discretization. Same as before with continuous piecewise linear \(\phi_h\) approximating \(\phi\).

Element by element mass lumping for discrete coupling energy:

\[
\sum_{T_j \subset T_h} \int_{T_j} I_h \left\{ s_h^2 \left[|\nabla \phi_h|^2 |n_h|^2 - (\nabla \phi_h \cdot n_h)^2\right] \right\}
\]

\(\Gamma\)-convergence: more involved because of \(\nabla \phi_h\) term.

Time-discrete stability!
Conclusion

- Computationally challenging with extreme parameters.
- Must resolve the degeneracy.
- Use a cutFEM approach instead of immersed boundary?
- Couple in more physical effects, such as electro-statics.
- Generalize to the **full Q**-tensor model.
- Shape optimization.
Final Remarks

- All simulations were implemented with the package **FELICITY**.
- MATLAB toolbox (with C++ behind it for speed).
- Or just google: “matlab felicity”.

Special thanks to NSF