A STRUCTURE PRESERVING FEM FOR UNIAXIAL NEMATIC LIQUID CRYSTALS

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Numerical Methods and New Perspectives for Extended Liquid Crystalline Systems
ICERM, December 9-14, 2019
Outline

The Landau - de Gennes Model

Structure Preserving FEM

Γ-Convergence

Discrete Gradient Flow

Simulations

Electric and Colloidal Effects

Conclusions and Open Problems
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Conclusions and Open Problems
Liquid Crystals with Variable Degree of Orientation

- **Nematic liquid crystal (LC)** molecules are often idealized as elongated rods. Modeling is further simplified by an averaging procedure to replace local arrangement of rods by a few order parameters.

![Left: Thermotropic LC; Right: Schlieren texture of liquid crystal nematic phase with surface point defects (boojums). Picture taken under a polarization microscope.](image)

- **Defects** are inherent to LC modeling, analysis and computation. They can be orientable (±1 degree) or non-orientable (±1/2 degree).

- **Computation** of LCs should allow for defects and yield convergent approximations of relevant physical quantities.
Half-integer order defects

Figure: Singularities (defects) of degree (b) $\frac{1}{2}$ and (c) $-\frac{1}{2}$. Taken from Sánchez et al., *Nature*, 2012.
**Orientability**

- Head-to-tail symmetry: **director fields** (unit vectors $n$) introduce an **orientational bias** into the model that is not physical (Ericksen’s model).

- Defects of degree $\pm 1/2$ are not orientable (cannot be described by director fields but rather by **line fields**); Landau-DeGennes model.
Ensemble Averaging

- **Probability distribution** \( \rho \): for \( x \in \Omega \) and \( p \in S^2 \) the unit sphere, \( \rho \) satisfies

\[
\rho(x, p) \geq 0, \quad \int_{S^2} \rho(x, p) ds(p) = 1, \quad \rho(x, p) = \rho(x, -p)
\]

- **First moment:**

\[
\int_{S^2} p \rho(x, p) ds(p) = -\int_{S^2} p \rho(x, -p) ds(p) = 0
\]

- **Second moment:**

\[
M(x) = \int_{S^2} p \otimes p \rho(x, p) ds(p) \in \mathbb{R}^{3 \times 3} \quad \Rightarrow \quad \text{tr}(M) = 1.
\]

- **Isotropic uniform distribution:**

\[
\rho(x, p) = \frac{1}{4\pi} \quad \Rightarrow \quad M = \frac{1}{3} I.
\]

- **The \( Q \)-tensor:** measures deviation from isotropic uniform distribution

\[
Q := M - \frac{1}{3} I, \quad \Rightarrow \quad Q = Q^T, \quad \text{tr}(Q) = 0.
\]
The $Q$-tensor

- **Biaxial form of $Q$:** for $n_1, n_2 \in S^2$ director fields and $s_1, s_2 \in \mathbb{R}$ scalar order parameters, $Q$ reads
  \[
  Q = s_1 \left( n_1 \otimes n_2 - \frac{1}{3} I \right) + s_2 \left( n_2 \otimes n_2 - \frac{1}{3} I \right)
  \]
  The signs of $n_1$ and $n_2$ have no effect on $Q$ (head-to-tail symmetry).

- **Eigenvalues $\lambda_i(Q)$ of $Q$:** probability distribution implies $-\frac{1}{3} \leq \lambda_i(Q) \leq \frac{2}{3}$
  \[
  \lambda_1(Q) = \frac{2s_1 - s_2}{3}, \quad \lambda_2(Q) = \frac{2s_2 - s_1}{3}, \quad \lambda_3(Q) = -\frac{s_1 + s_2}{3}
  \]

- **Uniaxial form of $Q$:** either $s_1 = 0$, $s_2 = 0$ or $s_1 = s_2$ and
  \[
  Q = s \left( n \otimes n - \frac{1}{3} I \right), \quad -\frac{1}{2} \leq s \leq 1.
  \]

A structure preserving FEM for uniaxial nematic liquid crystals
The One-Constant Landau - de Gennes Model

- **One-constant LdG energy**: sum of elastic and potential energies

\[ E[Q] := E_1[Q] + \frac{1}{\epsilon} E_2[Q] \]

where \( \epsilon > 0 \) is small (the nematic correlation length).

- **Elastic (Frank) energy**:

\[ E_1[Q] := \frac{1}{2} \int_\Omega |\nabla Q|^2 d\mathbf{x}. \]

- **Double-well potential energy**: \( E_2[Q] := \int_\Omega \psi(Q) d\mathbf{x} \) where

\[ \psi(Q) = A \text{tr}(Q^2) + B \text{tr}(Q^3) + C \text{tr}(Q^2)^2 \]

for \( A, B, C \in \mathbb{R} \). The minimizer of \( \psi(Q) \) is a uniaxial state.
Uniaxial vs Biaxial States

- **Biaxial:** for thermotropic LCs, the nematic biaxial phase remained *elusive* for a long period until
  - Acharya, et al, PRL, 2004;
  - Madsen, et al, PRL, 2004;

- **Uniaxial:** 2012 book by Sonnet and Virga (sec. 4.1) says
  
  *The vast majority of nematic liquid crystals do not, at least in homogeneous equilibrium states, show any sign of biaxiality.*

- **LdG-model:** does not enforce uniaxiality which, however, is still prevalent in many situations.

- **FEM:** we present a finite element method for uniaxial LCs.

- **Comparisons:** we compare uniaxial and biaxial behavior near a *Saturn-ring defect* at the end of this talk.
**$Q$-Model with Uniaxial Constraint**

- **One-constant energy:** $E[Q] = E_1[Q] + E_2[Q]$ where $Q = s(n \otimes n - \frac{1}{d} I)$

$$
E_1[Q] = \int_{\Omega} |\nabla Q|^2, \quad E_2[Q] = \int_{\Omega} \left( A \text{tr}(Q^2) + B \text{tr}(Q^3) + C \left(\text{tr}(Q^2)\right)^2\right).
$$

- **Property 1:**
  $$
  \nabla Q = \nabla s \otimes \left(\Theta - \frac{1}{d} I\right) + s \nabla \Theta, \quad \nabla \Theta : \Theta = \nabla \Theta : I = 0
  $$

  $$
  |\nabla Q|^2 = |\nabla s|^2 \left|\Theta - \frac{1}{d} I\right|^2 + s^2 |\nabla \Theta|^2 + 2s \nabla s \cdot \left[\nabla \Theta : \left(\Theta - \frac{1}{d} I\right)\right] \quad = \frac{d-1}{d} + 0.
  $$

- **Property 2:** A direct calculation gives

  $$
  s^2 = C_1 \text{tr}(Q^2), \quad s^3 = C_2 \text{tr}(Q^3), \quad s^4 = C_3 \left(\text{tr}(Q^2)\right)^2.
  $$

- **Equivalent one-constant energy:** $\kappa = \frac{d-1}{d}$, $\psi$ suitable double-well potential

  $$
  E_1[Q] = \int_{\Omega} \kappa |\nabla s|^2 + s^2 |\nabla \Theta|^2, \quad E_2[Q] = \int_{\Omega} \psi(s).
  $$
**Q-Model with Uniaxial Constraint**

- **One-constant energy:** \( E[Q] = E_1[Q] + E_2[Q] \) where \( Q = s \left( n \otimes n - \frac{1}{d} I \right) = \Theta \)

\[
E_1[Q] = \int_\Omega |\nabla Q|^2, \quad E_2[Q] = \int_\Omega \left( A \text{tr}(Q^2) + B \text{tr}(Q^3) + C \left( \text{tr}(Q^2) \right)^2 \right).
\]

- **Property 1:** \( \nabla Q = \nabla s \otimes \left( \Theta - \frac{1}{d} I \right) + s \nabla \Theta, \quad \nabla \Theta : \Theta = \nabla \Theta : I = 0 \)

\[
|\nabla Q|^2 = |\nabla s|^2 \left[ \Theta - \frac{1}{d} I \right]^2 + s^2 |\nabla \Theta|^2 + 2s \nabla s \cdot \left[ \nabla \Theta : \left( \Theta - \frac{1}{d} I \right) \right] = 0
\]

- **Property 2:** A direct calculation gives

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s^2 = C_1 \text{tr}(Q^2), \quad s^3 = C_2 \text{tr}(Q^3), \quad s^4 = C_3 \left( \text{tr}(Q^2) \right)^2.
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- **Equivalent one-constant energy:** \( \kappa = \frac{d-1}{d}, \psi \text{ suitable double-well potential} \)

\[
E_1[Q] = \int_\Omega \kappa |\nabla s|^2 + s^2 |\nabla \Theta|^2, \quad E_2[Q] = \int_\Omega \psi(s).
\]
One-Constant Ericksen’s Model

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

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

\[= E_1[s,n] + E_2[s]\]

where \(\kappa > 0\) and \(\psi\) is a double well potential with domain \((-\frac{1}{2}, 1)\).

- **Director field:** \(|n| = 1\) (unit vector).

- **Scalar order parameter:** \(s\) is the degree of orientation \((-\frac{1}{2} < s < 1)\).
  - \(s = 1\): perfect alignment with \(n\).
  - \(s = 0\): no preferred direction (isotropic). This defines the set of defects:
    \[S = \{x \in \Omega, \ s(x) = 0\}\]
  - \(s = -\frac{1}{2}\): perpendicular to \(n\).
**Ericksen Model vs. Oseen-Frank Model**

- When $s = s_0 > 0$, the energy reduces to the Oseen-Frank energy:

\[ E := \int_{\Omega} |\nabla n|^2 \, dx. \]

- One disadvantage of Oseen-Frank model is that the director field with finite energy is inconsistent with both line and plane defects.

  - **Line defects:**
    \[ n = \frac{r}{|r|}, \quad |\nabla n| = \frac{2}{|r|}. \]

  - Compute $\int_C |\nabla n|^2 \, dx$:
    \[ \int_0^1 \frac{4}{r^2} \, r \, dr = \infty. \]

  - Compute $\int_C \kappa |\nabla s|^2 + s^2 |\nabla n|^2 \, dx$:
    \[ \int_0^1 s^2 \frac{4}{r^2} \, r \, dr < \infty. \]

- Ericksen’s model allows for defects to have finite energy (regularization).
Ericksen Model vs. Oseen-Frank Model

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$$E := \int_\Omega |\nabla n|^2 \, dx.$$ 

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  - Compute $\int_C |\nabla n|^2 \, dx$:
    $$\int_0^1 \frac{4}{r^2} \, r \, dr = \infty.$$

  - Compute $\int_C \kappa |\nabla s|^2 + s^2 |\nabla n|^2 \, dx$:
    $$\int_0^1 s^2 \frac{4}{r^2} \, r \, dr < \infty.$$

- Ericksen’s model allows for defects to have finite energy (regularization).
Ericksen’s Model: Point Defect of Degree 1 in 2d

- Dirichlet boundary conditions: $s = s^*, \quad n = \frac{x}{|x|}$
- Director field: $\kappa = 2$
Ericksen’s Model: Point Defect of Degree 1 in 2d

- **Scalar order parameter**: $s_{\text{min}} = 2.02 \cdot 10^{-2}$

- **Movie**: Director field $n_h$ and order parameter $s_h$
\textbf{Q-Tensor Model: Point Defect of Degree 1 in 2d}

- **Dirichlet boundary conditions:** \( s = s^* , \quad n = \frac{x}{|x|} \)
- **Line field** \( \Theta = n \otimes n : \kappa = \frac{1}{2} \)
**Q-Tensor Model: Point Defect of Degree 1 in 2d**

- **Scalar order parameter** $s_h$: $s_{\text{min}} = 0.02$, $E_h = 9.18$

- **Movie:** Line field $\Theta_h$ and order parameter $s_h$
Q-Tensor Model: Point Defects of Degree $\pm1/2$ in 2d

- **Dirichlet boundary conditions**: $s = s^*$ corresponds to absolute minimum of double well potential $\psi$ and $n = n^*$ corresponds to defect of degree $3/2$ at $(0., 0.)$.

- **Scalar field $s$ and line field $\Theta = n \otimes n$:**

- **5 defects**: 4 defects of degree $\frac{1}{2}$ on the diagonals of $\Omega = (0, 1)^2$ and 1 defect of degree $-\frac{1}{2}$ at the origin.
Primary Goals

- **Structure preserving FEM**: Design discrete energies $E_h[Q_h] = E_h[\Theta_h, s_h]$ to approximate the Landau-deGennes energy

\[
E[\Theta, s] = \int_{\Omega} \kappa |\nabla s|^2 + s^2 |\nabla \Theta|^2 + \int_{\Omega} \psi(s) dx, \quad Q = s \left( n \otimes n - \frac{1}{d} I \right) = \Theta
\]

- **$\Gamma$-convergence**: if $Q_h$ are absolute minimizers of $E_h$

  - $Q_h$ converge to absolute minimizers $Q$ of $E$ as $h \to 0$
  - $E_h[Q_h] \to E[Q]$ as $h \to 0$.

- **Gradient flow**: Design a gradient flow to find a minimizer (equilibrium state or stationary point) $Q_h$ of the discrete energy $E_h$.

- **Monotonicity**: Energy decrease property of the gradient flow.

- **Simulation of defects**: Line and plane defects, saturn ring, degree $\pm 1$ and $\pm 1/2$ defects, etc (caused by electric fields and/or colloidal inclusions).
(Incomplete) Literature Review

Modeling and PDE
Ambrosio (1990)
Lin (1989, 1991)
Ball Zarnescu (2011); Ball Majumdar (2010).

Numerical methods for director fields:
Cohen Lin Luskin (1989)
Alouges (1997)
Liu Walkington (2000)
Calderer Golovaty Lin Liu (2002)
Bartels (2010); Bartels, Dolzmann, Nochetto (2012)
Yang Forest Li Liu Shen Wang (2013)

Numerical method for Ericksen’s model and $Q$-tensor model
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)
Bartels Raisch (2014)
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PDE Structure of Ericksen’s Model

- One constant model:

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

\[
\begin{align*}
\text{:=} & \ E_1[s, n] \\
\text{:=} & \ E_2[s]
\end{align*}
\]

Euler-Lagrange equation: (degenerate elliptic)

\[
\text{div} \ (s^2 \nabla n) - s^2 |\nabla n|^2 n = 0.
\]

\[-\kappa \Delta s - s |\nabla n|^2 + \frac{1}{2} \psi'(s) = 0.\]

- Energy identity: since $|n| = 1$, we have $\nabla |n|^2 = 2 n^T (\nabla n) = 0$.

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

- Equivalent energy: [Ambrosio 90, Lin 91] $E_1[s, n] = \tilde{E}_1[s, u]$ with

\[
\tilde{E}_1[s, u] := \int_{\Omega} (\kappa - 1) |\nabla s|^2 + |\nabla u|^2 \, dx, \quad (u = sn)
\]

i.e. a simple quadratic functional, but with a negative term ($\kappa < 1$).
**PDE Structure of Ericksen’s Model**

- **One constant model:**
  \[
  E[s, \mathbf{n}] := \int_{\Omega} \kappa |\nabla s|^2 + s^2 |\nabla \mathbf{n}|^2 \, dx + \int_{\Omega} \psi(s) \, dx \\
  := E_1[s, \mathbf{n}] + \int_{\Omega} \psi(s) \, dx := E_2[s]
  \]

  Euler-Lagrange equation: *(degenerate elliptic)*
  \[
  \text{div} \left( s^2 \nabla \mathbf{n} \right) - s^2 |\nabla \mathbf{n}|^2 \mathbf{n} = 0. \\
  - \kappa \Delta s - s |\nabla \mathbf{n}|^2 + \frac{1}{2} \psi'(s) = 0.
  \]

- **Energy identity:** since $|\mathbf{n}| = 1$, we have $\nabla |\mathbf{n}|^2 = 2 \mathbf{n}^T (\nabla \mathbf{n}) = 0$.
  \[
  \int_{\Omega} |\nabla (s \mathbf{n})|^2 \, dx = \int_{\Omega} |\mathbf{n} \otimes \nabla s + s \nabla \mathbf{n}|^2 \, dx = \int_{\Omega} |\nabla s|^2 + s^2 |\nabla \mathbf{n}|^2 \, dx.
  \]

- **Equivalent energy:** [Ambrosio 90, Lin 91] $E_1[s, \mathbf{n}] = \widetilde{E}_1[s, \mathbf{u}]$ with
  \[
  \widetilde{E}_1[s, \mathbf{u}] := \int_{\Omega} (\kappa - 1) |\nabla s|^2 + |\nabla \mathbf{u}|^2 \, dx, \quad (\mathbf{u} = s \mathbf{n})
  \]
  i.e. a simple quadratic functional, but with a negative term ($\kappa < 1$).
PDE Structure of the $Q$-Model: Relation to Ericksen’s Model

- **One-constant energy:** If $\kappa = \frac{d-1}{d}$ and $\psi$ is a suitable double-well potential, then
  \[
  E_1[Q] = \int_{\Omega} \kappa |\nabla s|^2 + s^2 |\nabla \Theta|^2, \quad E_2[Q] = \int_{\Omega} \psi(s).
  \]

- **Auxiliary variable:** If $U = s\Theta = s(n \otimes n)$, then
  \[
  \nabla U = \nabla s \otimes \Theta + s \nabla \Theta \quad \Rightarrow \quad |\nabla U|^2 = |\nabla s|^2 + s^2 |\nabla \Theta|^2
  \]
  because $\nabla \Theta : \Theta = 0$. Therefore $E_1[Q] = \tilde{E}_1[s, U]$ where
  \[
  \tilde{E}_1[s, U] = \int_{\Omega} (\kappa - 1) |\nabla s|^2 + |\nabla U|^2.
  \]

- **Structural conditions:**
  \[
  -\frac{1}{2} < s < 1, \quad U = s \underbrace{n \otimes n}_{=\Theta}, \quad n \in S^{d-1}.
  \]

- **Admissible class:**
  \[
  A := \{(s, U) \in H^1(\Omega) \times [H^1(\Omega)]^{d \times d} : (s, U) \text{ satisfy structural conditions a.e.}\}.
  \]
**PDE Structure of the $Q$-Model: Relation to Ericksen’s Model**

- **One-constant energy:** If $\kappa = \frac{d-1}{d}$ and $\psi$ is a suitable double-well potential, then
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  \nabla U = \nabla s \otimes \Theta + s \nabla \Theta \quad \Rightarrow \quad |\nabla U|^2 = |\nabla s|^2 + s^2 |\nabla \Theta|^2
  \]
  because $\nabla \Theta : \Theta = 0$. Therefore $E_1[Q] = \tilde{E}_1[s, U]$ where
  \[
  \tilde{E}_1[s, U] = \int_{\Omega} (\kappa - 1)|\nabla s|^2 + |\nabla U|^2.
  \]

- **Structural conditions:**
  \[\frac{-1}{2} < s < 1, \quad U = s n \otimes n, \quad n \in S^{d-1}.\]

- **Admissible class:**
  \[\mathbb{A} := \{(s, U) \in H^1(\Omega) \times [H^1(\Omega)]^{d \times d} : (s, U) \text{ satisfy structural conditions a.e.}\}.\]
Numerical Difficulties

- **PDEs:** Degenerate nonlinear elliptic PDEs.

- **Line field:** Construct a vector field $\Theta_h = n_n \otimes n_h$ such that $n_h$ has unit length at nodes (locking otherwise).

- **Scalar field:** Construct $s_h$ such that $-\frac{1}{2} < s_h < 1$ (at the nodes).

- **Auxiliary tensor field:** Construct a rank-one tensor field $U_h$ that satisfies the structural condition at the nodes $N_h$

$$U_h(x_i) = s_h(x_i) (n_h(x_i) \otimes n_h(x_i)) \quad \forall x_i \in N_h.$$

- **$\Gamma$-convergence:** theory without regularization that allows for defects.

- **Computation of minimizers:** discrete gradient flow.
Finite Element Spaces

- **Meshes:** Let $\mathcal{T}_h = \{T\}$ be a conforming, shape-regular triangulation of $\Omega$, with set of nodes (vertices) denoted by $N_h$.

- **Finite element spaces:**

  $\mathcal{U}_h := \{u_h \in [H^1(\Omega)]^d : u_h|_T \text{ is linear}\}$

  $\mathcal{S}_h := \{s_h \in H^1(\Omega) : s_h|_T \text{ is linear}\}$

  $\mathcal{N}_h := \{n_h \in \mathcal{U}_h : n_h|_T \text{ is linear} \}

  \quad |n_h(x_i)| = 1 \text{ at all nodes } x_i \in N_h\}

  $\mathcal{T}_h := N_h \otimes N_h$.

- **Weakly acute mesh:** the entries of the stiffness matrix $\{k_{ij}\}$ satisfy

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

  where $\{\phi_i\}$ denotes the continuous piecewise linear “hat” basis functions which satisfy $\phi_i(x_j) = \delta_{ij}$ for all nodes $x_j \in N_h$. 

A structure preserving FEM for uniaxial nematic liquid crystals

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Structure Preserving FEM

- **Dirichlet forms:** For a piecewise linear function $s_h$, we have

$$
\int_{\Omega} |\nabla s_h|^2 \, dx = \frac{1}{2} \sum_{i,j} k_{ij} (s_i - s_j)^2, \quad \int_{\Omega} |\nabla \Theta_h|^2 \, dx = \frac{1}{2} \sum_{i,j} k_{ij} (\Theta_i - \Theta_j)^2,
$$

where $s_i = s_h(x_i)$ and $\Theta_i = \Theta_h(x_i)$ for all nodes $x_i \in \mathcal{N}_h$.

- **Discrete energy:** approximate $E_1[s,\n] = \int_{\Omega} \kappa |\nabla s|^2 + s^2 |\nabla \Theta|^2 \, dx$ by

$$
E_1^h[s_h,\Theta_h] := \frac{\kappa}{2} \sum_{i,j=1}^{N} k_{ij} (s_i - s_j)^2 + \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left( \frac{s_i^2 + s_j^2}{2} \right) |\Theta_i - \Theta_j|^2.
$$

$$
\approx \int_{\Omega} s_h^2 |\nabla \Theta_h|^2 \, dx = \kappa \int_{\Omega} |\nabla s_h|^2 \, dx
$$

- **Nodal structural conditions:** let

$$
U_i = s_i \Theta_i = s_i (\mathbf{n}_i \otimes \mathbf{n}_i) \quad \forall x_i \in \mathcal{N}_h.
$$
Structure Preserving FEM

- **Dirichlet forms:** For a piecewise linear function $s_h$, we have
  \[
  \int_{\Omega} |\nabla s_h|^2 dx = \frac{1}{2} \sum_{i,j} k_{ij} (s_i - s_j)^2, \quad \int_{\Omega} |\nabla \Theta_h|^2 dx = \frac{1}{2} \sum_{i,j} k_{ij} (\Theta_i - \Theta_j)^2,
  \]
  where $s_i = s_h(x_i)$ and $\Theta_i = \Theta_h(x_i)$ for all nodes $x_i \in \mathcal{N}_h$.

- **Discrete energy:** approximate $E_1[s, \mathbf{n}] = \int_{\Omega} \kappa |\nabla s|^2 + s^2 |\nabla \Theta|^2 dx$ by
  \[
  E^h_1[s_h, \Theta_h] := \frac{\kappa}{2} \sum_{i,j=1}^{N} k_{ij} (s_i - s_j)^2 + \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left( \frac{s_i^2 + s_j^2}{2} \right) |\Theta_i - \Theta_j|^2.
  \]
  \[
  \approx \int_{\Omega} s_h^2 |\nabla \Theta_h|^2 dx
  \]
  \[
  = \kappa \int_{\Omega} |\nabla s_h|^2 dx
  \]

- **Nodal structural conditions:** let
  \[
  U_i = s_i \Theta_i = s_i (\mathbf{n}_i \otimes \mathbf{n}_i) \quad \forall x_i \in \mathcal{N}_h.
  \]
Stability of the Discrete Energy

- **Dirichlet form:** Let $u_h$ be piecewise linear with nodal values $U_i = s_i \Theta_i$

  \[
  2 \int_\Omega |\nabla U_h|^2 \, dx = \sum_{i,j} k_{ij} (s_i \Theta_i - s_j \Theta_j)^2
  \]

  \[
  = \sum_{i,j} k_{ij} \left( \frac{s_i + s_j}{2} (\Theta_i - \Theta_j) + (s_i - s_j) \frac{\Theta_i + \Theta_j}{2} \right)^2
  \]

- **Orthogonality:** Exploiting the relation $(\Theta_i - \Theta_j) \cdot (\Theta_i + \Theta_j) = 0$ yields

  \[
  2 \int_\Omega |\nabla U_h|^2 \, dx = \sum_{i,j} k_{ij} \left[ \left( \frac{s_i + s_j}{2} \right)^2 (\Theta_i - \Theta_j)^2 + (s_i - s_j)^2 \left( \frac{\Theta_i + \Theta_j}{2} \right)^2 \right]
  \]

  \[
  = \sum_{i,j} k_{ij} \frac{s_i^2 + s_j^2}{2} (\Theta_i - \Theta_j)^2 + \sum_{i,j} k_{ij} (s_i - s_j)^2 - \sum_{i,j} k_{ij} (s_i - s_j)^2 \left| \frac{\Theta_i - \Theta_j}{2} \right|^2
  \]

- **Energy inequalities:** $U_i = s_i \Theta_i$, $\tilde{s}_i = |s_i|$, $\tilde{U}_i = \tilde{s}_i \Theta_i$ (structural conditions)

  \[
  E^h_1[s_h, \Theta_h] \geq (\kappa - 1) \int_\Omega |\nabla s_h|^2 \, dx + \int_\Omega |\nabla U_h|^2 \, dx =: \tilde{E}^h_1[s_h, U_h]
  \]

  \[
  E^h_1[s_h, \Theta_h] \geq (\kappa - 1) \int_\Omega |\nabla \tilde{s}_h|^2 \, dx + \int_\Omega |\nabla \tilde{U}_h|^2 \, dx =: \tilde{E}^h_1[\tilde{s}_h, \tilde{U}_h].
  \]
Stability of the Discrete Energy

- **Dirichlet form:** Let $u_h$ be piecewise linear with nodal values $U_i = s_i \Theta_i$

  
  
  \[
  2 \int_\Omega |\nabla U_h|^2 \, dx = \sum_{i,j} k_{ij} (s_i \Theta_i - s_j \Theta_j)^2 \\
  = \sum_{i,j} k_{ij} \left( \frac{s_i + s_j}{2} (\Theta_i - \Theta_j) + (s_i - s_j) \frac{\Theta_i + \Theta_j}{2} \right)^2
  \]

- **Orthogonality:** Exploiting the relation $(\Theta_i - \Theta_j) : (\Theta_i + \Theta_j) = 0$ yields

  
  \[
  2 \int_\Omega |\nabla U_h|^2 \, dx = \sum_{i,j} k_{ij} \left[ \left( \frac{s_i + s_j}{2} \right)^2 (\Theta_i - \Theta_j)^2 + (s_i - s_j)^2 \left( \frac{\Theta_i + \Theta_j}{2} \right)^2 \right] \\
  = \sum_{i,j} k_{ij} \frac{s_i^2 + s_j^2}{2} (\Theta_i - \Theta_j)^2 + \sum_{i,j} k_{ij} (s_i - s_j)^2 \left( \frac{\Theta_i + \Theta_j}{2} \right)^2
  \]

- **Energy inequalities:** $U_i = s_i \Theta_i$, $\tilde{s}_i = |s_i|$, $\tilde{U}_i = \tilde{s}_i \Theta_i$ (structural conditions)

  \[
  E_1^h [s_h, \Theta_h] \geq (\kappa - 1) \int_\Omega |\nabla s_h|^2 \, dx + \int_\Omega |\nabla U_h|^2 \, dx =: \tilde{E}_1^h [s_h, U_h] \\
  E_1^h [\tilde{s}_h, \Theta_h] \geq (\kappa - 1) \int_\Omega |\nabla \tilde{s}_h|^2 \, dx + \int_\Omega |\nabla \tilde{U}_h|^2 \, dx =: \tilde{E}_1^h [\tilde{s}_h, \tilde{U}_h].
  \]
Discrete Admissible Class

- **Discrete structural conditions:**
  \[-\frac{1}{2} < s_i < 1, \quad U_i = s_i (n_i \otimes n_i), \quad |n_i| = 1 \quad \forall x_i \in N_h.\]

- **Discrete admissible class:**
  \[\mathbb{A}_h := \{(s_h, U_h) \in S_h \times U_h : (s_h, U_h) \text{ satisfies discrete structural conditions}\}.

- **Discrete restricted admissible class:**
  \[\mathbb{A}_h(I_hg, I_hR) := \{(s_h, U_h) \in A_h : s_h = I_hg, \quad U_h = I_hR \text{ on } \partial\Omega\},\]
  where \(I_h\) is the Lagrange interpolation operator.
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Assumptions for $\Gamma$-Convergence

- **Meshes:** Let $\{\mathcal{T}_h\}_{h \geq 0}$ be a sequence of weakly acute meshes.

- **Lim-sup inequality (consistency or recovery sequence):** Given $(s, U) \in \mathbb{A}$, namely $s, U = s \Theta \in H^1(\Omega)$, and satisfy Dirichlet boundary conditions $s = g, U = R$, there exists $(s_h, U_h) \in \mathbb{A}_h(I_h g, I_h R)$ such that $(s_h, U_h) \to (s, U)$ in $H^1(\Omega)$ and

  $$\limsup_{h \to 0} E^h_1[s_h, \Theta_h] \leq E_1[s, \Theta].$$

- **Lim-inf inequality (stability or lower semi-continuity):** Given a sequence $(s_h, U_h) \in \mathbb{A}_h(I_h g, I_h R)$, let $\tilde{s}_h = I_h |s_h|, \tilde{U}_h = I_h [\tilde{s}_h \Theta_h]$ be so that $(\tilde{s}_h, \tilde{U}_h)$ converges weakly in $H^1(\Omega)$ to $(\tilde{s}, \tilde{U})$. Then we have

  $$\tilde{E}_1[\tilde{s}, \tilde{U}] \leq \liminf_{h \to 0} \tilde{E}^h_1[\tilde{s}_h, \tilde{U}_h].$$

- **Equi-coercivity:** There exists a constant $C > 0$ such that

  $$\|s_h\|_{H^1(\Omega)}, \|U_h\|_{H^1(\Omega)} \leq CE^h_1[s_h, \Theta_h].$$
Theorem: $\Gamma$-Convergence for the $Q$-Model

Let $\{\mathcal{T}_h\}_{h \geq 0}$ be a sequence of weakly acute meshes. Then the discrete energy $E_h^s[s_h, \Theta_h]$ satisfies the lim-sup, lim-inf, and equi-coercivity properties. Moreover,

- If $E_h[s_h, \Theta_h] \leq \Lambda$ uniformly, then there exist subsequences (not relabeled) $(s_h, U_h)$, $(\tilde{s}_h, \tilde{U}_h)$, and $\Theta_h$ such that
  
  $\begin{align*}
  &\quad \text{\( \triangleright\)} \ (s_h, U_h) \text{ converges to } (s, U) \text{ weakly in } H^1 \text{ and strongly in } L^2; \\
  &\quad \text{\( \triangleright\)} \ (\tilde{s}_h, \tilde{U}_h) \text{ converges to } (\tilde{s}, \tilde{U}) \text{ weakly in } H^1 \text{ and strongly in } L^2; \\
  &\quad \text{\( \triangleright\)} \text{ The limits satisfy } \tilde{s} = |s| = |U| = |\tilde{U}|; \\
  &\quad \text{\( \triangleright\)} \text{ There exists a line field } \Theta \text{ defined in the complement of the singular set } S = \{s = 0\} \text{ such that } \Theta_h \text{ converges to } \Theta \text{ in } L^2(\Omega \setminus S) \text{ and } U = s\Theta \text{ and } \tilde{U} = \tilde{s}\Theta; \\
  &\quad \text{\( \triangleright\)} \Theta \text{ admits a Lebesgue gradient } \nabla \Theta \text{ and } |\nabla \tilde{U}|^2 = |\nabla \tilde{s}|^2 + \tilde{s}^2|\nabla \Theta|^2 \text{ a.e. in } \Omega \setminus S.
  \end{align*}$

- If $(s_h, \Theta_h)$ is a sequence of global minimizers of $E_h$, then every cluster point $(s, Q)$ is a global minimizer of $E$. 
Consistency or Recovery Sequence: Regularization of Functions in $\mathbb{A}(g, R)$

- **Regularization:** Given $\epsilon > 0$ and $(s, u) \in \mathbb{A}(g, R)$, i.e. satisfying $s = g$, $U = R$ on $\partial \Omega$, there exists $(s_\epsilon, U_\epsilon) \in \mathbb{A}(g, R) \cap [W^1_\infty(\Omega)]^{d+1}$ such that

$$
\|(s, U) - (s_\epsilon, U_\epsilon)\|_{H^1(\Omega)} \leq \epsilon.
$$

- **Difficulties:** pair $(s_\epsilon, U_\epsilon)$ must satisfy

  - **Structural conditions**

    $$
    \frac{1}{2} < s_\epsilon < 1, \quad \text{rank}(U_\epsilon) \leq 1, \quad \text{tr}(U_\epsilon) = s_\epsilon \quad \text{a.e. in } \Omega;
    $$

  - **Dirichlet boundary conditions**

    $$(s_\epsilon, U_\epsilon) = (g, R) \quad \text{on } \partial \Omega;$$

  - **Approximate** the pair $(s, U)$ in $H^1(\Omega)$.

- **Lim-sup equality:** For any $\epsilon > 0$, we obtain $(I_h s_\epsilon, I_h U_\epsilon) \in \mathbb{A}_h(I_h g, I_h R)$ by nodewise interpolation of $(s_\epsilon, U_\epsilon)$ and

$$
E_1[s_\epsilon, \Theta_\epsilon] = \lim_{h \to 0} E^h_1[I_h s_\epsilon, I_h \Theta_\epsilon] = \lim_{h \to 0} \tilde{E}^h_1[I_h s_\epsilon, I_h U_\epsilon] = \tilde{E}_1[s_\epsilon, U_\epsilon].
$$
Consistency or Recovery Sequence: Regularization of Functions in $\mathbb{A}(g, R)$

- **Regularization:** Given $\epsilon > 0$ and $(s, u) \in \mathbb{A}(g, R)$, i.e. satisfying $s = g$, $U = R$ on $\partial \Omega$, there exists $(s_\epsilon, U_\epsilon) \in \mathbb{A}(g, R) \cap [W^1_{\infty}(\Omega)]^{d+1}$ such that
  \[
  \| (s, U) - (s_\epsilon, U_\epsilon) \|_{H^1(\Omega)} \leq \epsilon.
  \]

- **Difficulties:** pair $(s_\epsilon, U_\epsilon)$ must satisfy
  - **Structural conditions**
    \[-\frac{1}{2} < s_\epsilon < 1, \quad \text{rank}(U_\epsilon) \leq 1, \quad \text{tr}(U_\epsilon) = s_\epsilon \quad \text{a.e. in } \Omega;\]
  - **Dirichlet boundary conditions**
    \[(s_\epsilon, U_\epsilon) = (g, R) \quad \text{on } \partial \Omega;\]
  - **Approximate** the pair $(s, U)$ in $H^1(\Omega)$.

- **Lim-sup equality:** For any $\epsilon > 0$, we obtain $(I_h s_\epsilon, I_h U_\epsilon) \in \mathbb{A}_h(I_h g, I_h R)$ by nodewise interpolation of $(s_\epsilon, U_\epsilon)$ and
  \[
  E_1[s_\epsilon, \Theta_\epsilon] = \lim_{h \to 0} E^h_1[I_h s_\epsilon, I_h \Theta_\epsilon] = \lim_{h \to 0} \tilde{E}^h_1[I_h s_\epsilon, I_h U_\epsilon] = \tilde{E}_1[s_\epsilon, U_\epsilon].
  \]
Weak Lower Semi-continuity: Lim-Inf Inequality

- **Energy inequality:** Recall that

\[
E^h_1[s_h, \Theta_h] \geq \tilde{E}^h_1[\tilde{s}_h, \tilde{U}_h] = -\frac{1}{d} \int_{\Omega} |\nabla \tilde{s}_h|^2 \, dx + \int_{\Omega} |\nabla \tilde{U}_h|^2 \, dx,
\]

where \(\tilde{s}_h = I_h |s_h|\) and \(\tilde{u}_h = I_h [\tilde{s}_h \Theta_h]\).

- **Difficulties:** is the right-hand side convex in \(\nabla \tilde{U}_h\)? Note negative first term!
  
  ▶ True if \(|\tilde{s}_h| = |\tilde{U}_h|\) in \(\Omega\)
  
  ▶ But this relation \(|\tilde{s}_h(x_i)| = |\tilde{U}_h(x_i)|\) is only valid at the nodes \(x_i \in N_h\).

- **Weak lower semi-continuity:** Let \(W_h\) in \(U_h\) converge weakly to \(W\) in the \(H^1\)-norm. Then

\[
\lim_{h \to 0} \inf \int_{\Omega} -\frac{1}{d} |\nabla I_h|W_h|^2 + |\nabla W_h|^2 \geq \int_{\Omega} -\frac{1}{d} |\nabla W|^2 + |\nabla W|^2.
\]
Weak Lower Semi-continuity: Lim-Inf Inequality

- **Energy inequality:** Recall that

\[
E_1^h [s_h, \Theta_h] \geq \tilde{E}_1^h [\tilde{s}_h, \tilde{U}_h] = -\frac{1}{d} \int_\Omega |\nabla \tilde{s}_h|^2 dx + \int_\Omega |\nabla \tilde{U}_h|^2 dx,
\]

where \( \tilde{s}_h = I_h |s_h| \) and \( \tilde{u}_h = I_h [\tilde{s}_h \Theta_h] \).

- **Difficulties:** is the right-hand side convex in \( \nabla \tilde{U}_h \)? Note negative first term!
  - True if \( |\tilde{s}_h| = |\tilde{U}_h| \) in \( \Omega \)
  - But this relation \( |\tilde{s}_h(x_i)| = |\tilde{U}_h(x_i)| \) is only valid at the nodes \( x_i \in N_h \).

- **Weak lower semi-continuity:** Let \( W_h \) in \( U_h \) converge weakly to \( W \) in the \( H^1 \)-norm. Then

\[
\liminf_{h \to 0} \int_\Omega -\frac{1}{d} |\nabla I_h |W_h||^2 + |\nabla W_h|^2 \geq \int_\Omega -\frac{1}{d} |\nabla W||^2 + |\nabla W|^2.
\]
Equi-Coercivity

For any \((s_h, U_h) \in \mathbb{A}_h(I_hg, I_hR)\) we have \(U_h = I_h[s_h \Theta_h], \tilde{U}_h = I_h[\tilde{s}_h \Theta_h]\) and

- **Estimate for** \((s_h, U_h):\)

\[
E^h_1[s_h, \Theta_h] \geq \frac{d - 1}{d} \max \left\{ \int_\Omega |\nabla U_h|^2, \int_\Omega |\nabla s_h|^2 \right\}
\]

- **Estimate for** \((\tilde{s}_h, \tilde{U}_h):\)

\[
E^h_1[\tilde{s}_h, \Theta_h] \geq \frac{d - 1}{d} \max \left\{ \int_\Omega |\nabla \tilde{U}_h|^2, \int_\Omega |\nabla \tilde{s}_h|^2 \right\}.
\]
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Discrete Gradient Flow for the $Q$-Model

- **Three-step algorithm:** Given $s = s_h$ and $\Theta = \Theta_h = I_h [n_h \otimes n_h]$, iterate
  
  ▶ **Weighted gradient flow for $\Theta$:** find $T_k = n_k \otimes t_k + t_k \otimes n_k$ such that $t_k$ is tangent to $n_k$ and for all $v$ tangent to $n_k$ (Bartels, Raisch (2014))

  \[
  \frac{1}{\tau} \int_{\Omega} s_k^2 \nabla t_k : \nabla v + t_k \cdot v + \delta E^h_1 [s_k, \Theta_k + T_k; V] = 0 \quad \forall V = n_k \otimes v + v \otimes n_k.
  \]

  ▶ **Projection:** update $\Theta$ by

  \[
  \Theta_{k+1} := \frac{n_k + t_k}{|n_k + t_k|} \otimes \frac{n_k + t_k}{|n_k + t_k|}.
  \]

  ▶ **Gradient flow for $s$:** find $s_{k+1}$ such that

  \[
  \frac{1}{2\tau} \int_{\Omega} |s_{k+1} - s_k|^2 + \delta s E^h_1 [s_{k+1}, \Theta_{k+1}; z] + \delta s E^h_2 [s_{k+1}; z] = 0 \quad \forall z,
  \]

  where $\delta s E_2 [s; z] = \int_{\Omega} \psi'(s)z$ and $\psi$ is a double-well potential.

- **Relaxation:** the effect of weight $s^2_k$ is to allow for larger variations of $t_k$. 

A structure preserving FEM for uniaxial nematic liquid crystals
Discrete Gradient Flow for the $Q$-Model

- **Three-step algorithm:** Given $s = s_h$ and $\Theta = \Theta_h = I_h [n_h \otimes n_h]$, iterate

  - **Weighted gradient flow for $\Theta$:** find $T_k = n_k \otimes t_k + t_k \otimes n_k$ such that $t_k$ is tangent to $n_k$ and for all $v$ tangent to $n_k$ (Bartels, Raisch (2014))

    $$
    \frac{1}{\tau} \int_{\Omega} s_k^2 \nabla t_k : \nabla v + t_k \cdot v + \delta_\Theta E^h_1 [s_k, \Theta_k + T_k; V] = 0 \quad \forall V = n_k \otimes v + v \otimes n_k.
    $$

  - **Projection:** update $\Theta$ by

    $$
    \Theta_{k+1} := \frac{n_k + t_k}{|n_k + t_k|} \otimes \frac{n_k + t_k}{|n_k + t_k|}.
    $$

  - **Gradient flow for $s$:** find $s_{k+1}$ such that

    $$
    \frac{1}{2\tau} \int_{\Omega} |s_{k+1} - s_k|^2 + \delta_s E^h_1 [s_{k+1}, \Theta_{k+1}; z] + \delta_s E^h_2 [s_{k+1}; z] = 0 \quad \forall z,
    $$

    where $\delta_s E_2 [s; z] = \int_{\Omega} \psi'(s)z$ and $\psi$ is a double-well potential.

- **Relaxation:** the effect of weight $s_k^2$ is to allow for larger variations of $t_k$. 

A structure preserving FEM for uniaxial nematic liquid crystals

Ricardo H. Nochetto
Energy Decrease Property for the $Q$-Model

- **Variations in line field:** avoid nonlinear term $t \otimes t$ (Bartels & Raisch 2014).

- **Projection step:** is energy decreasing (Alouges 1997, Bartels 2010).

- **Convex splitting:** to treat the double-well potential term in the gradient flow for $s_k$.

- **Theorem (energy decrease property)** If the meshes $\mathcal{T}_h$ are weakly acute and the time step $\tau \leq C_0 h^{d/2}$, then there holds

  $$E_1^h[s_N, \Theta_N] + \frac{2}{\tau} \sum_{k=0}^{N-1} \left( \| s_k \nabla t_k \|_{L^2(\Omega)}^2 + \| t_k \|_{L^2(\Omega)}^2 + \| s_{k+1} - s_k \|^2 \right)$$

  $$\leq E_1^h[s_0, \Theta_0] \quad \forall N \geq 1.$$

  Thus, the algorithm stops in a finite number of steps for any tolerance $\varepsilon$. 
Why do we have a CFL condition?

- **Tangential variations:** In Step 1 we update \( \Theta_k = I_h(n_k \otimes n_k) \) according to

\[
\Theta_k + T_k, \quad T_k = n_k \otimes t_k + t_k \otimes n_k
\]

with \( t_k(x_i) \cdot n_k(x_i) = 0 \) (nodal tangential update).

- **Rank-one update:** In Step 2 we create the rank-1 update

\[
(n_k + t_k) \otimes (t_k + n_k) = \Theta_k + T_k + t_k \otimes t_k
\]

and next normalize it (projection into discrete line fields update).

- **Correction term:** We must thus account for \( t_k \otimes t_k \)

\[
\sum_{i,j} k_{ij} \left( s_k(x_i)^2 + s_k(x_j)^2 \right) |\delta_{ij}(t_k \otimes t_k)|^2 \approx h^{-d} \left( \int_{\Omega} s_k^2 |\nabla t_k|^2 + |t_k|^2 \right)^2.
\]

An induction argument together with \( \tau \leq C_0 h^{d/2} \), with \( C_0 \) proportional to \( E_h[s_0, \Theta_0] \), allows for control of this term.
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Ericksen’s Model: “Propeller” Defect $\kappa = 0.1$

- **Director field at 4 slices:** $z = 0.2, 0.4, 0.6, 0.8$

- **Movie:** Director field at $z = 0$

- **Movie:** 3d defect is marked in red.
Q-Model: 3-D Line Defect of Degree 1

- **Line field at 4 slices:** \( z = 0.1, 0.35, 0.65, 0.9; \) \( s_{\text{min}} = 1.0 \times 10^{-2} \).

- **Movie:** Line field at \( z = 0.5 \). Gradient flow starts with line defect of degree 1 located at \((0.25, 0.25)\).
Q-Model: 3-D Line Defect of Degree $1/2$

- **Line field at 4 slices:** $z = 0.1, 0.35, 0.65, 0.9$; $s_{\text{min}} = 6.8 \times 10^{-2}$.

- **Movie:** Line field at $z = 0.5$. Gradient flow starts with line defect of degree $1$ at $(0.25, 0.25)$. 
Twisting Defect: Non-Orientable Line Defect of Degree $+\frac{1}{2}$ in a Cube

- **Computation of line field and line defect**: Horizontal slices of the $+1/2$ degree line defect at levels $z = 0.0, 0.5, 1.0$ colored by scalar field $s$. The non-straight defect is the $s = 0.05$ iso-surface.

- **Movie**: Display of line field at levels $z = 0.0, 0.5, 1.0$ colored by scalar field.
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Electric Field Effect with \( Q \)-Model: Freedericksz Transition

- **Electric energy:** let \( E \) be a given (fixed) external field,

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

Above, \( K_{ext} \) is a weight parameter, and \( \bar{\varepsilon}, \gamma_a, \varepsilon_a \) are material constants.

- **Simulation:** Freedericksz transition with Dirichlet boundary conditions on the left and right of \( \Omega \) and zero Neumann condition on top and bottom of \( \Omega \). The electric field is \( E = (1, 0)^\top \).
Colloidal Inclusion Effect with $Q$-Model

- **Immersed boundary method:** to avoid mesh-acuteness issues (conforming meshes are hard to construct).

- **Phase-field approach:** $\phi \approx 0$ inside the colloid and $\phi \approx 1$ in the LC region.

- **Weak anchoring energy:** penalization of $(s, \Theta) = (s^*, \nu \otimes \nu)$ on colloidal surface with unit normal $\nu$

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

- **Movie:** 2d simulation. Spherical colloid with center $(0.5, 0.7)^T$ and radius 0.2. Dirichlet boundary conditions: $s = s^*, \Theta = n \otimes n$ with $n$ normal to the colloid on its surface and $n = n^* = (1,0)$ on $\partial \Omega$.

- **Two defects of degree $-1/2$:** located on top and bottom of colloid.
3d Saturn Ring Defect with $Q$-Model

- **Setting:** Dirichlet boundary conditions $\Theta = (0, 0, 1) \otimes (0, 0, 1)$ and $s = s^*$ in $\Omega = [0, 1]^3$. A colloid of radius 0.25 is located at the center of the domain.

- **Defect of degree $-1/2$:** analysis by S. Alama, L. Bronsard, X. Lamy (2016).

- **Movie:** Evolution of order parameter $s$
Saturn Ring Defect: Degree of Biaxiality (Majumdar-Zarnescu, S. Walker)

\[
0 \leq \beta(Q) = 1 - 6 \frac{(\text{tr}Q^3)^2}{(\text{tr}Q^2)^3} \leq 1 \quad \Rightarrow \quad \begin{cases} 
\beta(Q) = 0 & \text{uniaxial} \\
\beta(Q) = 1 & \text{biaxial}
\end{cases}
\]

Figure (a): Measure of biaxiality \( \beta(Q) \) (blue (uniaxial), red (biaxial));
Figure (b): plot of the function \(|Q_{LdG} - Q_{uni}|\) (the error can be up to 15-20%).
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Conclusions

- **Structure preserving FEMs** for the one constant Ericksen’s model

\[
E[s, n] := \int_{\Omega} \kappa |\nabla s|^2 + s^2 |\nabla n|^2 \, dx + \int_{\Omega} \psi(s) \, dx, \quad \kappa > 0.
\]

and the Landau-DeGennes \( Q \)-tensor model \((Q = s n \otimes n)\)

\[
E[Q] = \int_{\Omega} \kappa |\nabla s|^2 + s^2 |\nabla \Theta|^2 + \int_{\Omega} \psi(s), \quad \kappa = \frac{d-1}{d} < 1.
\]

- **\( \Gamma \)-convergence** of the FEM for any dimension \( d \): convergence of global discrete minimizers to global minimizers.

- **Monotone energy decrease** of the quasi-gradient and weighted gradient flows.

- **High dimensional defects** can be captured by our FEMs for both models.

- **2d and 3d electric and colloidal effects**: comparisons between Ericksen and Landau-deGennes models. **Computations done within Matlab software FELICITY (S. Walker (2017)).**
Open Problems

- Explore alternatives to the gradient flow such as direct minimization.
- $\Gamma$-convergence to local minimizers.
- Error estimates.
- Comparison of uniaxial $Q$-model with the full (biaxial) $Q$-model.
- Coupling of the $Q$-model with incompressible fluids.

Publications: