A STRUCTURE PRESERVING FEM FOR UNIAXIAL NEMATIC LIQUID CRYSTALS

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Numerical Methods and New Perspectives
for Extended Liquid Crystalline Systems
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Outline

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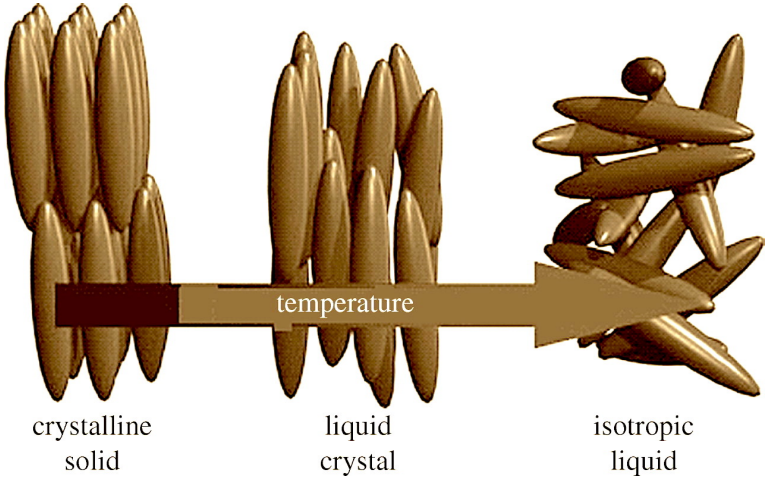
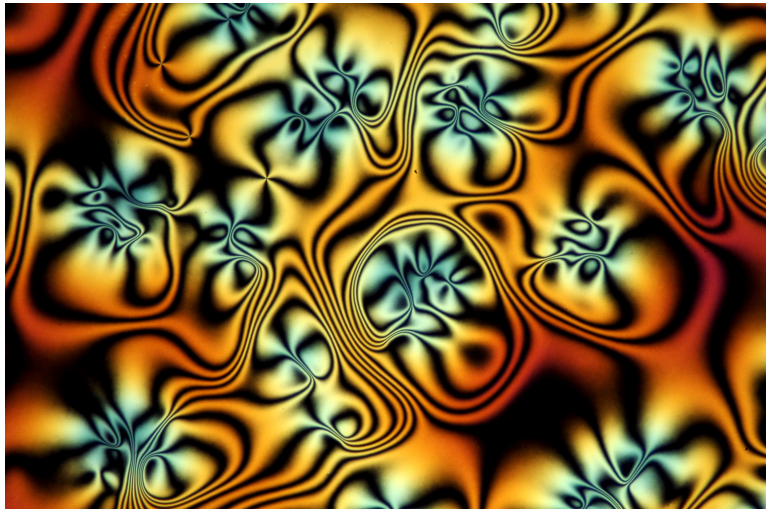
Liquid Crystals with Variable Degree of Orientation

- **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.

- **Defects** are inherent to LC modeling, analysis and computation. They can be orientable (± 1 degree) or non-orientable ($\pm 1/2$ degree).
- **Computation** of LCs should allow for defects and yield convergent approximations of relevant physical quantities.

Half-integer order defects

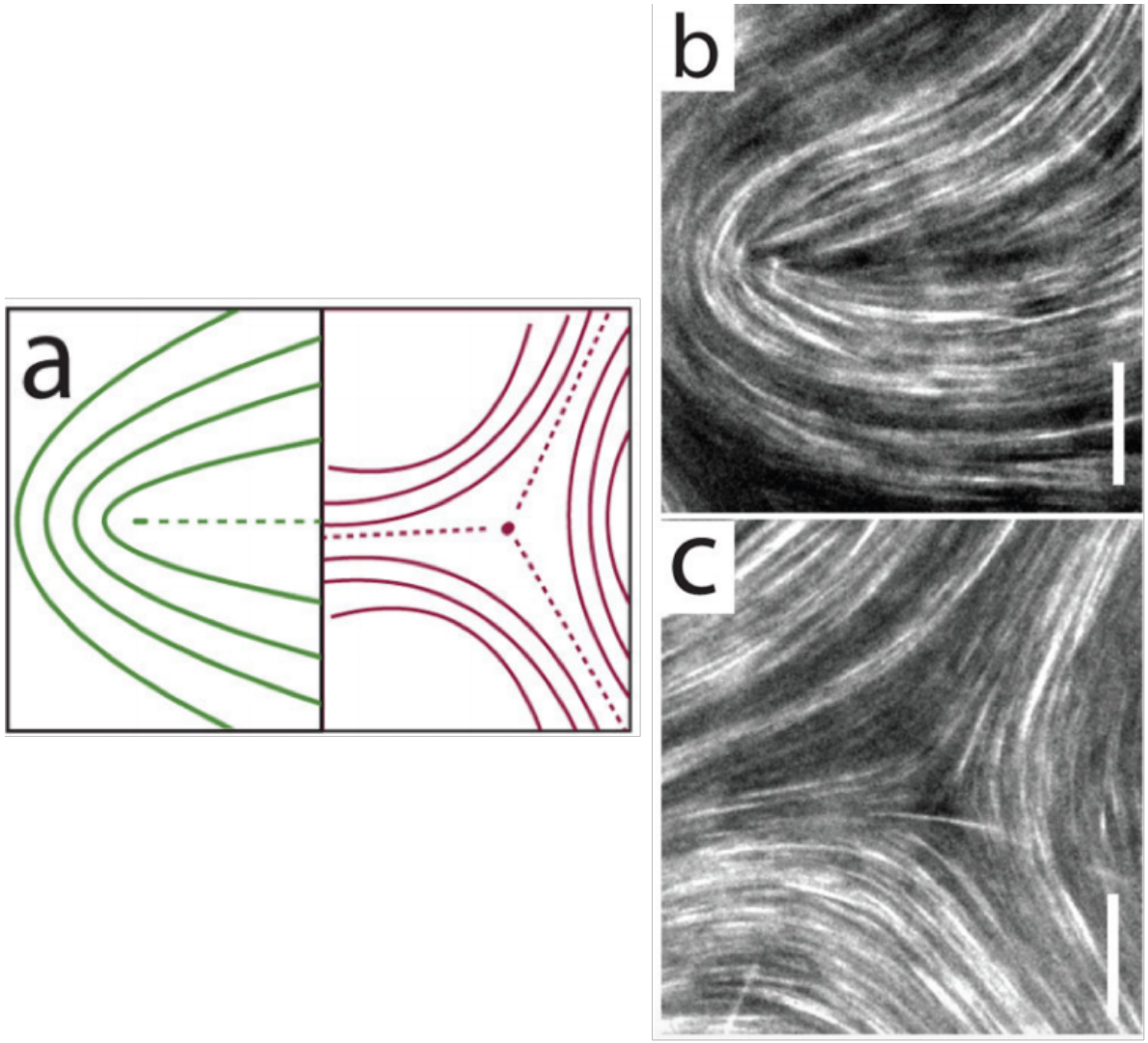
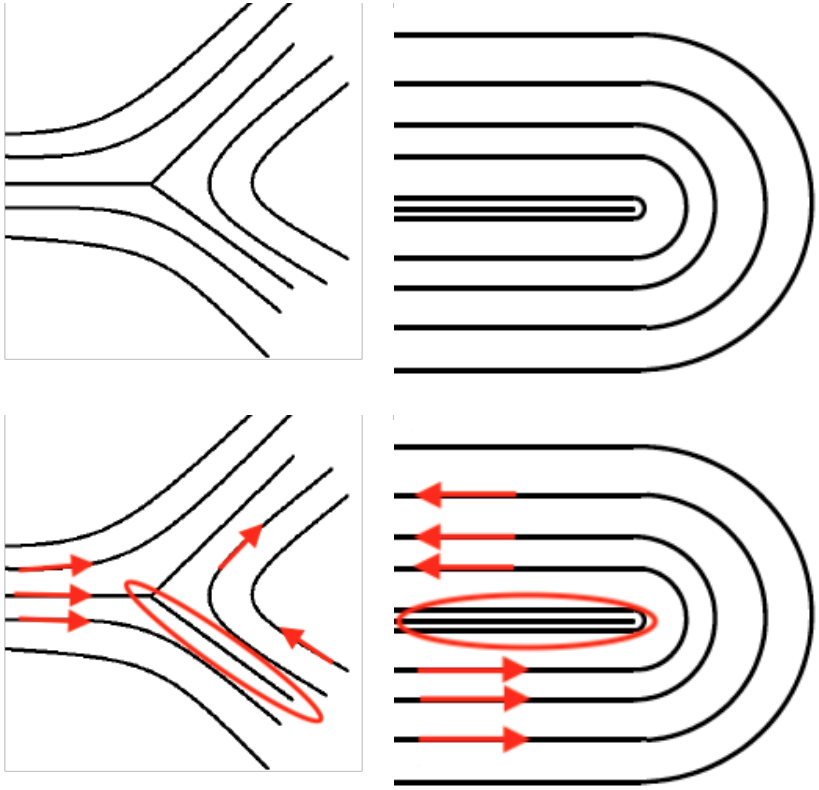


Figure: Singularities (defects) of degree (b) $1/2$ and (c) $-1/2$. Taken from Sánchez et al., *Nature*, 2012.

Orientability

- Head-to-tail symmetry: director fields (unit vectors $\boldsymbol{n}$) 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 ρ:** for $\mathbf{x} \in \Omega$ and $\mathbf{p} \in \mathbb{S}^2$ the unit sphere, ρ satisfies

$$\rho(\mathbf{x},\mathbf{p}) \geq 0, \qquad \int_{\mathbb{S}^2} \rho(\mathbf{x},\mathbf{p}) ds(\mathbf{p}) = 1, \qquad \rho(\mathbf{x},\mathbf{p}) = \rho(\mathbf{x},-\mathbf{p})$$

- **First moment:** $\int_{\mathbb{S}^2} \mathbf{p}\, \rho(\mathbf{x},\mathbf{p}) ds(\mathbf{p}) = -\int_{\mathbb{S}^2} \mathbf{p}\, \rho(\mathbf{x},-\mathbf{p}) ds(\mathbf{p}) = 0$

- **Second moment:**

$$\mathbf{M}(\mathbf{x}) = \int_{\mathbb{S}^2} \mathbf{p} \otimes \mathbf{p}\, \rho(\mathbf{x},\mathbf{p}) ds(\mathbf{p}) \in \mathbb{R}^{3\times 3} \qquad \Rightarrow \qquad \mathrm{tr}(\mathbf{M}) = 1.$$

- **Isotropic uniform distribution:**

$$\rho(\mathbf{x},\mathbf{p}) = \frac{1}{4\pi} \qquad \Rightarrow \qquad \mathbf{M} = \frac{1}{3}\mathbf{I}.$$

- **The $\boldsymbol{Q}$-tensor:** measures deviation from isotropic uniform distribution

$$\boldsymbol{Q} := \mathbf{M} - \frac{1}{3}\mathbf{I}, \qquad \Rightarrow \qquad \boldsymbol{Q} = \boldsymbol{Q}^T, \quad \mathrm{tr}(\boldsymbol{Q}) = 0.$$

The Q-tensor

- **Biaxial form of $\mathbf{Q}$:** for $\mathbf{n}_1, \mathbf{n}_2 \in \mathbb{S}^2$ director fields and $s_1, s_2 \in \mathbb{R}$ scalar order parameters, $\mathbf{Q}$ reads

$$\mathbf{Q} = s_1\Big(\mathbf{n}_1 \otimes \mathbf{n}_2 - \frac{1}{3}\mathbf{I}\Big) + s_2\Big(\mathbf{n}_2 \otimes \mathbf{n}_2 - \frac{1}{3}\mathbf{I}\Big)$$

The signs of $\mathbf{n}_1$ and $\mathbf{n}_2$ have no effect on $\mathbf{Q}$ (head-to-tail symmetry).

- **Eigenvalues $\lambda_i(\mathbf{Q})$ of $\mathbf{Q}$:** probability distribution implies $-\frac{1}{3} \le \lambda_i(\mathbf{Q}) \le \frac{2}{3}$

$$\lambda_1(\mathbf{Q}) = \frac{2s_1 - s_2}{3}, \qquad \lambda_2(\mathbf{Q}) = \frac{2s_2 - s_1}{3} \qquad \lambda_3(\mathbf{Q}) = -\frac{s_1 + s_2}{3}$$

- **Uniaxial form of $\mathbf{Q}$:** either $s_1 = 0$, $s_2 = 0$ or $s_1 = s_2$ and

$$\mathbf{Q} = s\Big(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\Big), \qquad -\frac{1}{2} \le s \le 1.$$

The One-Constant Landau - de Gennes Model

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

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

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

- **Elastic (Frank) energy:**

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

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

$$\psi(\mathbf{Q}) = A \operatorname{tr}(\mathbf{Q}^2) + B \operatorname{tr}(\mathbf{Q}^3) + C \operatorname{tr}(\mathbf{Q}^2)^2$$

for $A, B, C \in \mathbb{R}$. The minimizer of $\psi(\mathbf{Q})$ 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;
  - Prasad, et al, J. Amer. Chem. Soc., 2005.

- **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:** $E[\boldsymbol{Q}] = E_1[\boldsymbol{Q}] + E_2[\boldsymbol{Q}]$ where $\boldsymbol{Q} = s(\underbrace{\boldsymbol{n}\otimes\boldsymbol{n}}_{=\Theta} - \frac{1}{d}I)$

$$E_1[\boldsymbol{Q}] = \int_\Omega |\nabla \boldsymbol{Q}|^2, \quad E_2[\boldsymbol{Q}] = \int_\Omega \Big(A\ \mathrm{tr}(\boldsymbol{Q}^2) + B\ \mathrm{tr}(\boldsymbol{Q}^3) + C\ \big(\mathrm{tr}(\boldsymbol{Q}^2)\big)^2\Big).$$

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

$$|\nabla \boldsymbol{Q}|^2 = |\nabla s|^2 \underbrace{\Big|\boldsymbol{\Theta} - \frac{1}{d}\boldsymbol{I}\Big|^2}_{=\frac{d-1}{d}} + s^2|\nabla\boldsymbol{\Theta}|^2 + 2s\nabla s \cdot \underbrace{\Big[\nabla\boldsymbol{\Theta} : \Big(\boldsymbol{\Theta} - \frac{1}{d}\boldsymbol{I}\Big)\Big]}_{=0}.$$

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

$$s^2 = C_1 \mathrm{tr}(\boldsymbol{Q}^2), \quad s^3 = C_2 \mathrm{tr}(\boldsymbol{Q}^3), \quad s^4 = C_3\big(\mathrm{tr}(\boldsymbol{Q}^2)\big)^2.$$

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

$$E_1[\boldsymbol{Q}] = \int_\Omega \kappa|\nabla s|^2 + s^2|\nabla\Theta|^2, \quad E_2[\boldsymbol{Q}] = \int_\Omega \psi(s).$$

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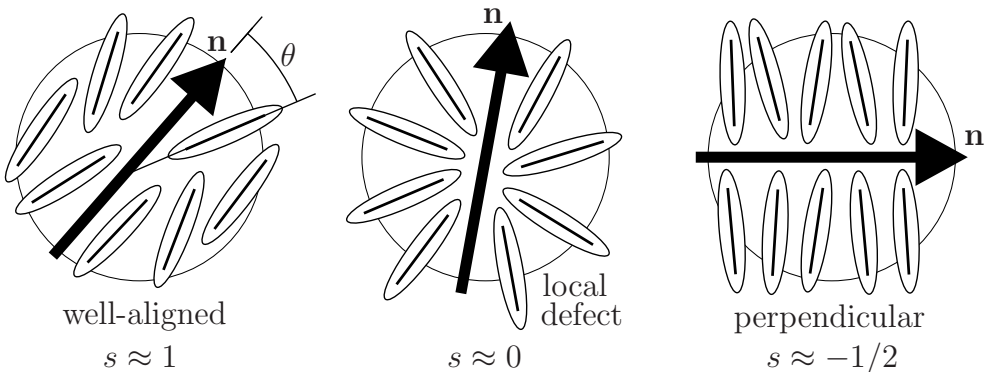
One-Constant Ericksen's Model

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

$$E[s,\boldsymbol{n}] := \underbrace{\int_\Omega \kappa|\nabla s|^2 + s^2|\nabla \boldsymbol{n}|^2 dx}_{:=E_1[s,\boldsymbol{n}]} + \underbrace{\int_\Omega \psi(s)dx}_{:=E_2[s]}$$

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

- **Director field:** $|\boldsymbol{n}| = 1$ (unit vector).



- **Scalar order parameter:** s is the **degree of orientation** $(-1/2 < s < 1)$.
  - $s = 1$: perfect alignment with $\boldsymbol{n}$.
  - $s = 0$: no preferred direction (isotropic). This defines the **set of defects**:

$$\mathcal{S} = \{x \in \Omega, \quad s(x) = 0\}.$$

  - $s = -1/2$: perpendicular to $\boldsymbol{n}$.

Ericksen Model vs. Oseen-Frank Model

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

$$E := \int_\Omega |\nabla \boldsymbol{n}|^2 dx.$$

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

- Line defects:

$$\boldsymbol{n} = \frac{\boldsymbol{r}}{|\boldsymbol{r}|}, \quad |\nabla \boldsymbol{n}| = \frac{2}{|\boldsymbol{r}|}.$$

- Compute $\int_C |\nabla \boldsymbol{n}|^2 dx$:

$$\int_0^1 \frac{4}{r^2}\, r dr = \infty.$$

- Compute $\int_C \kappa |\nabla s|^2 + s^2 |\nabla \boldsymbol{n}|^2 dx$:

$$\int_0^1 s^2 \frac{4}{r^2}\, r dr < \infty.$$

- Ericksen's model allows for defects to have finite energy (regularization).

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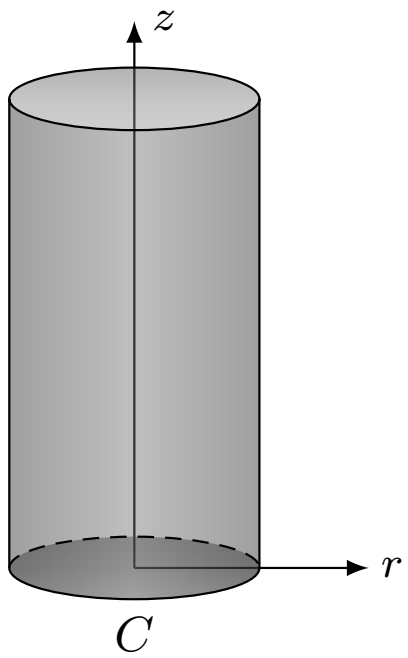

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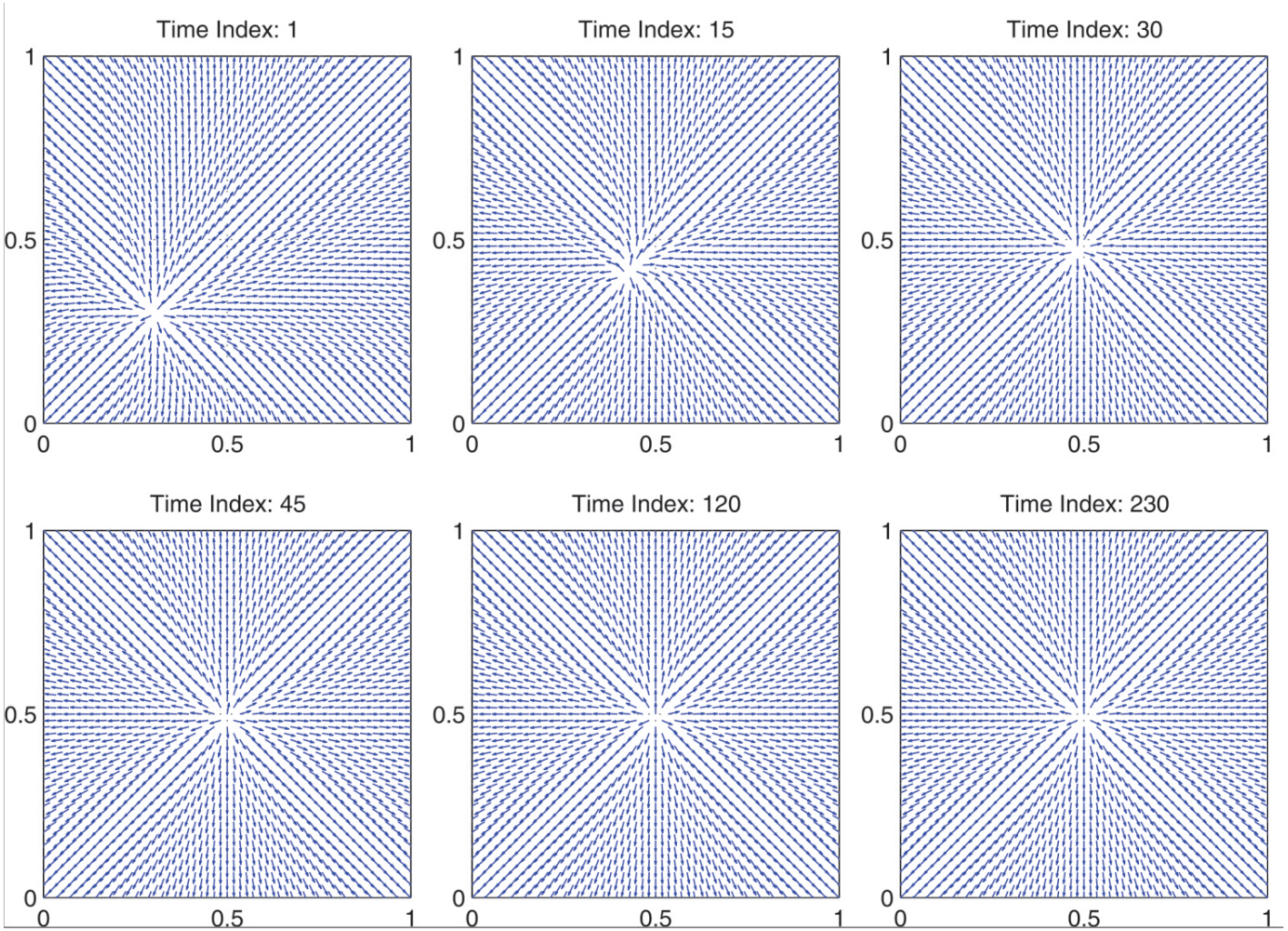
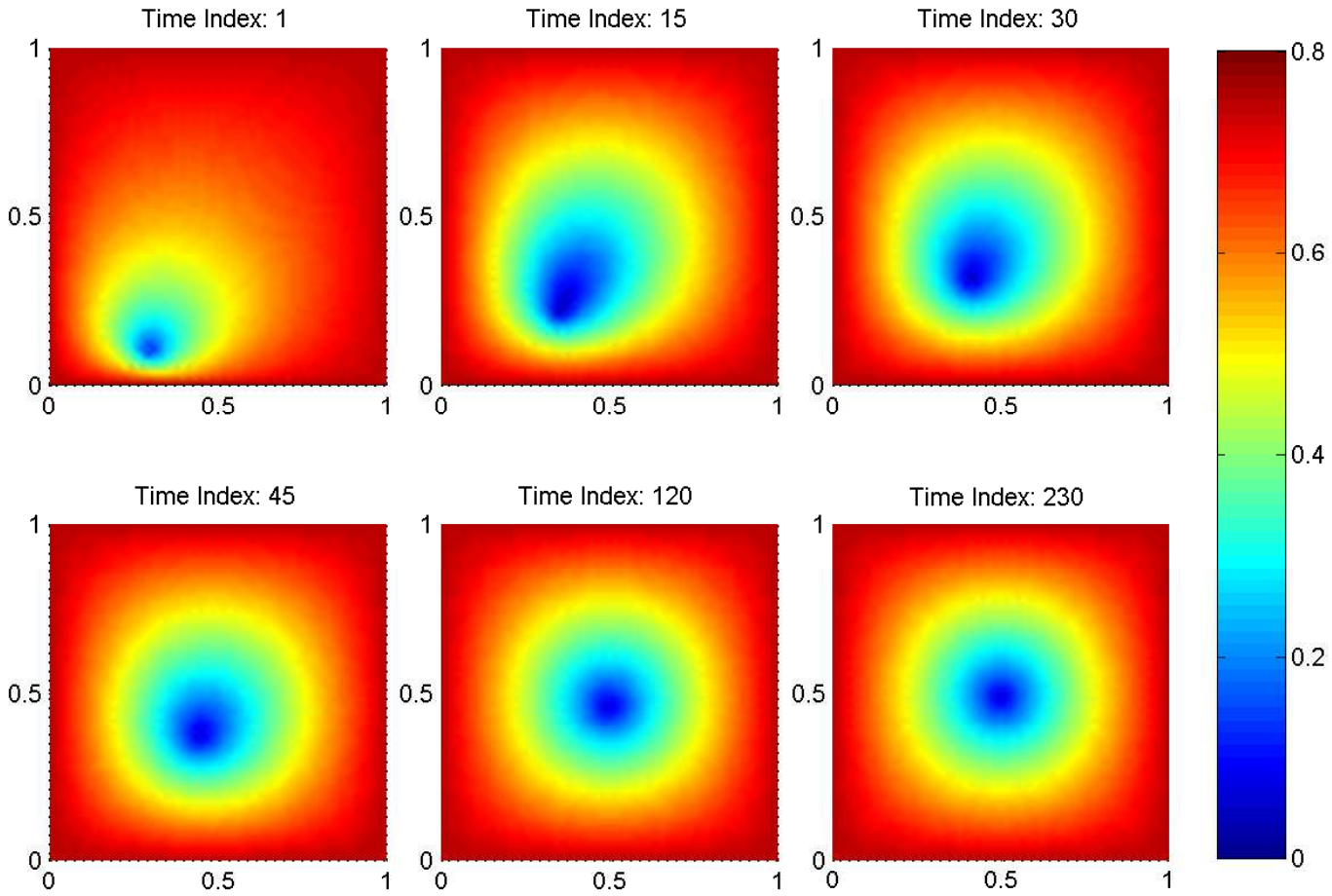
Ericksen's Model: Point Defect of Degree 1 in 2d

- **Dirichlet boundary conditions:** $s = s^*, \quad \boldsymbol{n} = \frac{\boldsymbol{x}}{|\boldsymbol{x}|}$
- **Director field:** $\kappa = 2$



Ericksen's Model: Point Defect of Degree 1 in 2d

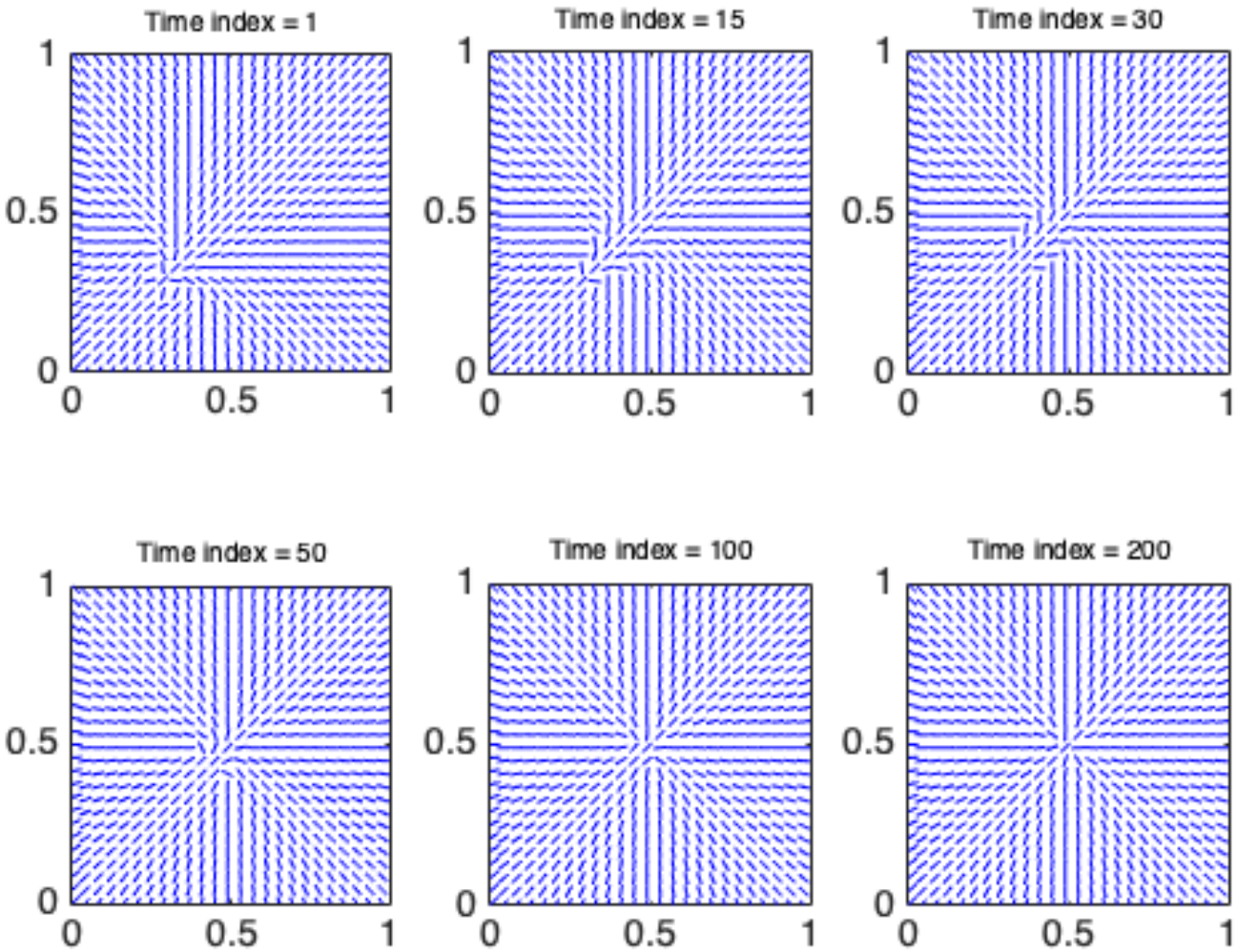
- **Scalar order parameter:** $s_{\min} = 2.02 \cdot 10^{-2}$



- **Movie:** Director field $\boldsymbol{n}_h$ and order parameter s_h

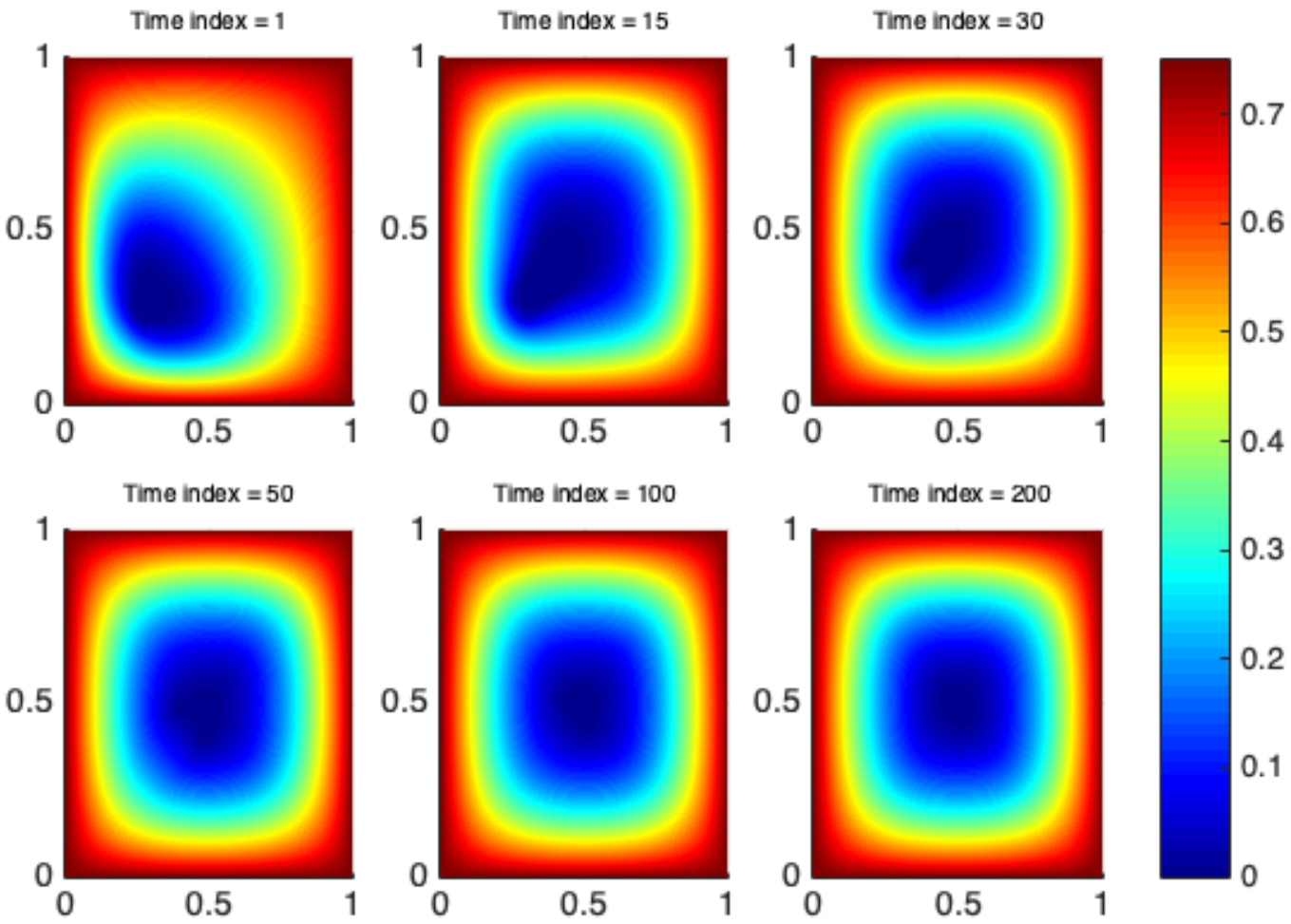
Q-Tensor Model: Point Defect of Degree 1 in 2d

- **Dirichlet boundary conditions:** $s = s^*, \quad \boldsymbol{n} = \frac{\boldsymbol{x}}{|\boldsymbol{x}|}$
- **Line field** $\boldsymbol{\Theta} = \boldsymbol{n} \otimes \boldsymbol{n}$**:** $\kappa = \frac{1}{2}$



Q-Tensor Model: Point Defect of Degree 1 in 2d

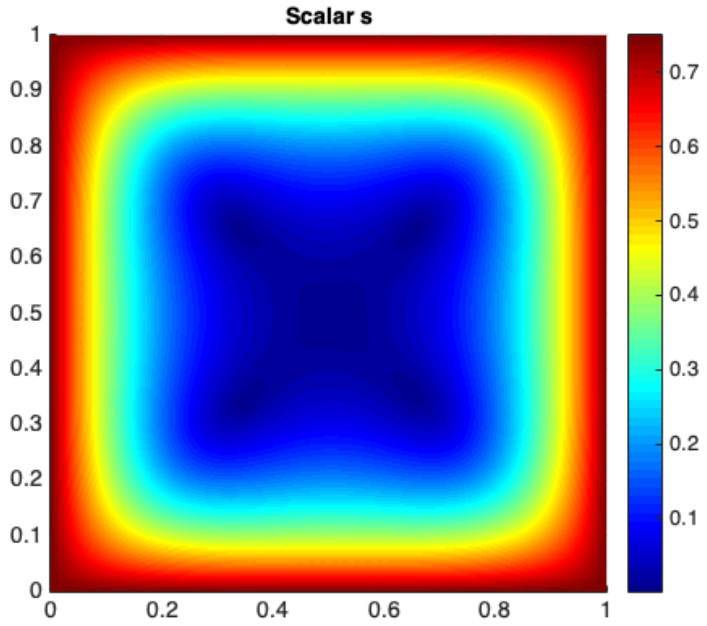
- **Scalar order parameter** s_h**:** $s_{\min} = 0.02, E_h = 9.18$

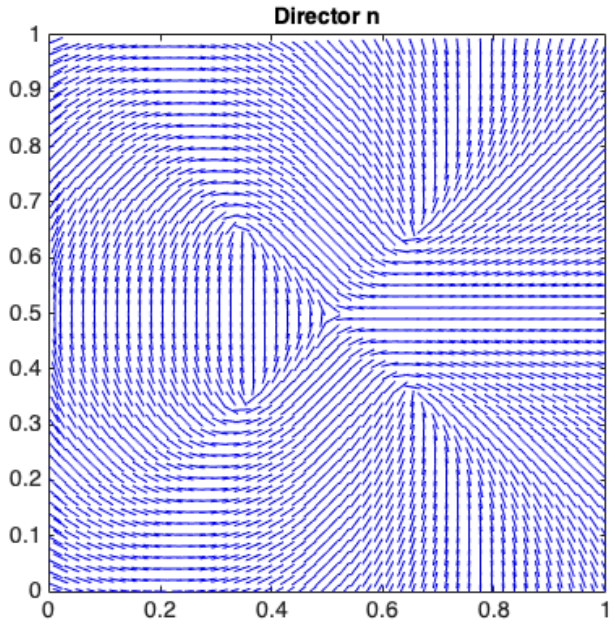


- **Movie:** Line field $\mathbf{\Theta}_h$ and order parameter s_h

Q-Tensor Model: Point Defects of Degree $\pm 1/2$ in 2d

- **Dirichlet boundary conditions:** $s = s^*$ corresponds to absolute minimum of double well potential ψ and $\boldsymbol{n} = \boldsymbol{n}^*$ corresponds to defect of degree $3/2$ at $(0., 0.)$.
- **Scalar field s and line field $\boldsymbol{\Theta} = \boldsymbol{n} \otimes \boldsymbol{n}$:**





- **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 $E_h[\mathbf{Q}_h] = E_h[\mathbf{\Theta}_h, s_h]$ to approximate the Landau-deGennes energy

$$E[\mathbf{\Theta}, s] = \underbrace{\int_\Omega \kappa|\nabla s|^2 + s^2|\nabla \mathbf{\Theta}|^2}_{=E_2[\mathbf{Q}]} + \underbrace{\int_\Omega \psi(s)dx}_{=E_2[s]}, \quad \boldsymbol{Q} = s\Big(\underbrace{\boldsymbol{n}\otimes\boldsymbol{n}}_{=\mathbf{\Theta}} - \frac{1}{d}\boldsymbol{I}\Big)$$

- Γ-convergence: if $\boldsymbol{Q}_h$ are absolute minimizers of E_h
  - $\boldsymbol{Q}_h$ converge to absolute minimizers $\boldsymbol{Q}$ of E as $h \to 0$
  - $E_h[\boldsymbol{Q}_h] \to E[\boldsymbol{Q}]$ as $h \to 0$.
- Gradient flow: Design a gradient flow to find a minimizer (equilibrium state or stationary point) $\boldsymbol{Q}_h$ of the discrete energy E_h.
- Monotonicity: Energy decrease property of the gradient flow.
- Simulation of defects: Line and plane defects, saturn ring, degree ± 1 and $\pm 1/2$ defects, etc (caused by electric fields and/or colloidal inclusions).

(Incomplete) Literature Review

Modeling and PDE
Hardt Kinderlehrer Lin (1986), Kinderlehrer (1991), Kinderlehrer, Ou (1992)
Brezis (1987, 1989), Ericksen (1991)
Virga (1994), DeGennes-Prost (1995)
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)
Lin Lin Wang (2010)
Bartels Raisch (2014)
Walkington (2011, 2017).

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PDE Structure of Ericksen's Model

- **One constant model:**

$$E[s,\boldsymbol{n}] := \underbrace{\int_\Omega \kappa|\nabla s|^2 + s^2|\nabla \boldsymbol{n}|^2 dx}_{:=E_1[s,\boldsymbol{n}]} + \underbrace{\int_\Omega \psi(s)dx}_{:=E_2[s]}$$

Euler-Lagrange equation: (degenerate elliptic)

$$\text{div}\,(s^2\nabla \boldsymbol{n}) - s^2|\nabla \boldsymbol{n}|^2\boldsymbol{n} = 0.$$

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

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

$$\int_\Omega |\nabla \underbrace{(s\boldsymbol{n})}_{:=\boldsymbol{u}}|^2 dx = \int_\Omega |\boldsymbol{n}\otimes\nabla s + s\nabla \boldsymbol{n}|^2 dx = \int_\Omega |\nabla s|^2 + s^2|\nabla \boldsymbol{n}|^2 dx.$$

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

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

i.e. a simple quadratic functional, but with a negative term ($\kappa < 1$).

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PDE Structure of the Q-Model: Relation to Ericksen's Model

- **One-constant energy:** If $\kappa = \frac{d-1}{d}$ and ψ is a suitable double-well potential, then

$$E_1[\boldsymbol{Q}] = \int_\Omega \kappa |\nabla s|^2 + s^2 |\nabla \Theta|^2, \quad E_2[\boldsymbol{Q}] = \int_\Omega \psi(s).$$

- **Auxiliary variable:** If $\boldsymbol{U} = s\boldsymbol{\Theta} = s\big(\boldsymbol{n} \otimes \boldsymbol{n}\big)$, then

$$\nabla \boldsymbol{U} = \nabla s \otimes \boldsymbol{\Theta} + s \nabla \boldsymbol{\Theta} \quad \Rightarrow \quad |\nabla \boldsymbol{U}|^2 = |\nabla s|^2 + s^2 |\nabla \Theta|^2$$

because $\nabla \boldsymbol{\Theta} : \boldsymbol{\Theta} = 0$. Therefore $E_1[\boldsymbol{Q}] = \widetilde{E}_1[s, \boldsymbol{U}]$ where

$$\widetilde{E}_1[s, \boldsymbol{U}] = \int_\Omega (\kappa - 1)|\nabla s|^2 + |\nabla \boldsymbol{U}|^2.$$

- **Structural conditions:**

$$-\frac{1}{2} < s < 1, \qquad \boldsymbol{U} = s \underbrace{\mathbf{n} \otimes \mathbf{n}}_{=\Theta}, \qquad \mathbf{n} \in \mathbb{S}^{d-1}.$$

- **Admissible class:**

$$\mathbb{A} := \big\{ (s, \boldsymbol{U}) \in H^1(\Omega) \times [H^1(\Omega)]^{d \times d} : \ (s, \boldsymbol{U}) \text{ satisfy structural conditions a.e.} \big\}.$$

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Numerical Difficulties

- **PDEs:** Degenerate nonlinear elliptic PDEs.
- **Line field:** Construct a vector field $\mathbf{\Theta}_h = \mathbf{n}_n \otimes \mathbf{n}_h$ such that $\mathbf{n}_h$ 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 $\mathbf{U}_h$ that satisfies the structural condition at the nodes $\mathcal{N}_h$

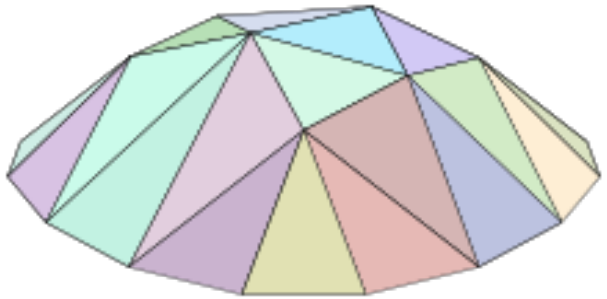
$$\mathbf{U}_h(x_i) = s_h(x_i)\big(\mathbf{n}_h(x_i) \otimes \mathbf{n}_h(x_i)\big) \qquad \forall\, x_i \in \mathcal{N}_h.$$

- **Γ-convergence:** theory without regularization that allows for defects.
- **Computation of minimizers:** discrete gradient flow.

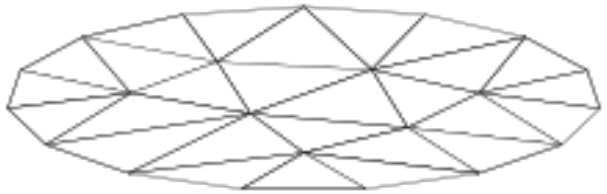
Finite Element Spaces

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

- **Finite element spaces:**



$$\mathbb{U}_h := \{\boldsymbol{u}_h \in [H^1(\Omega)]^d : \boldsymbol{u}_h|_T \text{ is linear}\}$$
$$\mathbb{S}_h := \{s_h \in H^1(\Omega) : s_h|_T \text{ is linear}\}$$
$$\mathbb{N}_h := \{\boldsymbol{n}_h \in \mathbb{U}_h : \boldsymbol{n}_h|_T \text{ is linear}$$
$$|\boldsymbol{n}_h(x_i)| = 1 \text{ at all nodes } x_i \in \mathcal{N}_h\}$$
$$\mathbb{T}_h := \mathbb{N}_h \otimes \mathbb{N}_h.$$



- **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 $x_j \in \mathcal{N}_h$.

Structure Preserving FEM

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

$$\int_\Omega |\nabla s_h|^2 dx = \frac{1}{2}\sum_{i,j} k_{ij}(s_i - s_j)^2, \quad \int_\Omega |\nabla \mathbf{\Theta}_h|^2 dx = \frac{1}{2}\sum_{i,j} k_{ij}(\mathbf{\Theta}_i - \mathbf{\Theta}_j)^2,$$

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

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

$$E_1^h[s_h, \mathbf{\Theta}_h] := \underbrace{\frac{\kappa}{2}\sum_{i,j=1}^N k_{ij}\,(s_i - s_j)^2}_{=\kappa\int_\Omega |\nabla s_h|^2 dx} + \underbrace{\frac{1}{2}\sum_{i,j=1}^N k_{ij}\left(\frac{s_i^2 + s_j^2}{2}\right)|\mathbf{\Theta}_i - \mathbf{\Theta}_j|^2}_{\approx\int_\Omega s_h^2|\nabla \mathbf{\Theta}_h|^2 dx}.$$

- **Nodal structural conditions:** let

$$\boldsymbol{U}_i = s_i\mathbf{\Theta}_i = s_i\big(\mathbf{n}_i \otimes \mathbf{n}_i\big) \quad \forall x_i \in \mathcal{N}_h.$$

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Stability of the Discrete Energy

- **Dirichlet form:** Let $\boldsymbol{u}_h$ be piecewise linear with nodal values $\boldsymbol{U}_i = s_i \boldsymbol{\Theta}_i$

$$2\int_\Omega |\boldsymbol{\nabla} \boldsymbol{U}_h|^2 dx = \sum_{i,j} k_{ij} (s_i \boldsymbol{\Theta}_i - s_j \boldsymbol{\Theta}_j)^2$$

$$= \sum_{i,j} k_{ij} \left(\frac{s_i + s_j}{2} (\boldsymbol{\Theta}_i - \boldsymbol{\Theta}_j) + (s_i - s_j) \frac{\boldsymbol{\Theta}_i + \boldsymbol{\Theta}_j}{2} \right)^2$$

- **Orthogonality:** Exploiting the relation $(\boldsymbol{\Theta}_i - \boldsymbol{\Theta}_j) : (\boldsymbol{\Theta}_i + \boldsymbol{\Theta}_j) = 0$ yields

$$2\int_\Omega |\boldsymbol{\nabla} \boldsymbol{U}_h|^2 dx = \sum_{i,j} k_{ij} \left[\left(\frac{s_i + s_j}{2} \right)^2 (\boldsymbol{\Theta}_i - \boldsymbol{\Theta}_j)^2 + (s_i - s_j)^2 \left(\frac{\boldsymbol{\Theta}_i + \boldsymbol{\Theta}_j}{2} \right)^2 \right]$$

$$= \sum_{i,j} k_{ij} \frac{s_i^2 + s_j^2}{2} (\boldsymbol{\Theta}_i - \boldsymbol{\Theta}_j)^2 + \sum_{i,j} k_{ij} (s_i - s_j)^2 - \sum_{i,j} k_{ij} (s_i - s_j)^2 \left| \frac{\boldsymbol{\Theta}_i - \boldsymbol{\Theta}_j}{2} \right|^2$$

- **Energy inequalities:** $\boldsymbol{U}_i = s_i \boldsymbol{\Theta}_i$, $\widetilde{s}_i = |s_i|$, $\widetilde{\boldsymbol{U}}_i = \widetilde{s}_i \boldsymbol{\Theta}_i$ (structural conditions)

$$E_1^h[s_h, \boldsymbol{\Theta}_h] \geq (\kappa - 1) \int_\Omega |\nabla s_h|^2 dx + \int_\Omega |\nabla \boldsymbol{U}_h|^2 dx =: \widetilde{E}_1^h[s_h, \boldsymbol{U}_h]$$

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$$E_1^h[s_h, \boldsymbol{\Theta}_h] \geq (\kappa - 1) \int_\Omega |\nabla \widetilde{s}_h|^2 dx + \int_\Omega |\nabla \widetilde{\boldsymbol{U}}_h|^2 dx =: \widetilde{E}_1^h[\widetilde{s}_h, \widetilde{\boldsymbol{U}}_h].$$

Discrete Admissible Class

- **Discrete structural conditions:**

$$-\frac{1}{2} < s_i < 1, \quad \boldsymbol{U}_i = s_i\big(\mathbf{n}_i \otimes \mathbf{n}_i\big), \quad |\mathbf{n}_i| = 1 \qquad \forall x_i \in \mathcal{N}_h.$$

- **Discrete admissible class:**

$$\mathbb{A}_h := \big\{(s_h, \boldsymbol{U}_h) \in \mathbb{S}_h \times \mathbb{U}_h : \ (s_h, \mathbf{U}_h) \ \text{ satisfies discrete structural conditions}\big\}.$$

- **Discrete restricted admissible class:**

$$\mathbb{A}_h(I_h g, I_h \boldsymbol{R}) := \big\{(s_h, \boldsymbol{U}_h) \in \mathbb{A}_h : \quad s_h = I_h g, \quad \boldsymbol{U}_h = I_h \boldsymbol{R} \ \text{ on } \partial\Omega\big\},$$

where I_h is the Lagrange interpolation operator.

Outline

Assumptions for Γ-Convergence

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

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

$$\limsup_{h\to 0} E_1^h[s_h, \boldsymbol{\Theta}_h] \leq E_1[s, \boldsymbol{\Theta}].$$

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

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

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

$$\|s_h\|_{H^1(\Omega)}, \|\boldsymbol{U}_h\|_{H^1(\Omega)} \leq C E_1^h[s_h, \boldsymbol{\Theta}_h].$$

Theorem: Γ-Convergence for the Q-Model

Let $\{\mathcal{T}_h\}_{h\geq 0}$ be a sequence of weakly acute meshes. Then the discrete energy $E_1^h[s_h, \boldsymbol{\Theta}_h]$ satisfies the lim-sup, lim-inf, and equi-coercivity properties. Moreover,

- If $E_h[s_h, \boldsymbol{\Theta}_h] \leq \Lambda$ uniformly, then there exist subsequences (not relabeled) $(s_h, \boldsymbol{U}_h)$, $(\tilde{s}_h, \tilde{\boldsymbol{U}}_h)$, and $\boldsymbol{\Theta}_h$ such that
  - $(s_h, \boldsymbol{U}_h)$ converges to $(s, \boldsymbol{U})$ weakly in H^1 and strongly in L^2;
  - $(\tilde{s}_h, \tilde{\boldsymbol{U}}_h)$ converges to $(\tilde{s}, \tilde{\boldsymbol{U}})$ weakly in H^1 and strongly in L^2;
  - The limits satisfy $\tilde{s} = |s| = |\boldsymbol{U}| = |\tilde{\boldsymbol{U}}|$;
  - There exists a line field $\boldsymbol{\Theta}$ defined in the complement of the singular set $\mathcal{S} = \{s = 0\}$ such that $\boldsymbol{\Theta}_h$ converges to $\boldsymbol{\Theta}$ in $L^2(\Omega \setminus \mathcal{S})$ and $\boldsymbol{U} = s\boldsymbol{\Theta}$ and $\tilde{\boldsymbol{U}} = \tilde{s}\boldsymbol{\Theta}$;
  - Θ admits a Lebesgue gradient $\nabla\boldsymbol{\Theta}$ and $|\nabla\widetilde{U}|^2 = |\nabla\widetilde{s}|^2 + \widetilde{s}^2|\nabla\boldsymbol{\Theta}|^2$ a.e. in $\Omega \setminus \mathcal{S}$.
- If $(s_h, \boldsymbol{\Theta}_h)$ is a sequence of global minimizers of E_h, then every cluster point $(s, \boldsymbol{Q})$ is a global minimizer of E.

Consistency or Recovery Sequence: Regularization of Functions in $\mathbb{A}(g, \boldsymbol{R})$

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

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

- **Difficulties:** pair $(s_\epsilon, \boldsymbol{U}_\epsilon)$ must satisfy
  - **Structural conditions**

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

  - **Dirichlet boundary conditions**

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

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

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

$$E_1[s_\epsilon, \boldsymbol{\Theta}_\epsilon] = \lim_{h \to 0} E_1^h[I_h s_\epsilon, I_h \boldsymbol{\Theta}_\epsilon] = \lim_{h \to 0} \widetilde{E}_1^h[I_h s_\epsilon, I_h \boldsymbol{U}_\epsilon] = \widetilde{E}_1[s_\epsilon, \boldsymbol{U}_\epsilon].$$

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Weak Lower Semi-continuity: Lim-Inf Inequality

- **Energy inequality:** Recall that

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

where $\widetilde{s}_h = I_h|s_h|$ and $\widetilde{\boldsymbol{u}}_h = I_h[\widetilde{s}_h \boldsymbol{\Theta}_h]$.

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

- **Weak lower semi-continuity:** Let $\boldsymbol{W}_h$ in $\mathbb{U}_h$ converge weakly to $\boldsymbol{W}$ in the H^1-norm. Then

$$\liminf_{h\to 0} \int_\Omega -\frac{1}{d}\left|\nabla I_h|\boldsymbol{W}_h|\right|^2 + |\nabla \boldsymbol{W}_h|^2 \geq \int_\Omega -\frac{1}{d}\left|\nabla|\boldsymbol{W}|\right|^2 + |\nabla \boldsymbol{W}|^2.$$

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Equi-Coercivity

For any $(s_h, \boldsymbol{U}_h) \in \mathbb{A}_h(I_h g, I_h \boldsymbol{R})$ we have $\boldsymbol{U}_h = I_h[s_h \boldsymbol{\Theta}_h]$, $\widetilde{\boldsymbol{U}}_h = I_h[\widetilde{s}_h \boldsymbol{\Theta}_h]$ and

- **Estimate for $(s_h, \boldsymbol{U}_h)$:**

$$E_1^h[s_h, \boldsymbol{\Theta}_h] \geq \frac{d-1}{d} \max\left\{\int_\Omega |\nabla \boldsymbol{U}_h|^2, \int_\Omega |\nabla s_h|^2\right\}$$

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Outline

Discrete Gradient Flow for the Q-Model

- **Three-step algorithm:** Given $s = s_h$ and $\boldsymbol{\Theta} = \boldsymbol{\Theta}_h = I_h[\boldsymbol{n}_h \otimes \boldsymbol{n}_h]$, iterate
  - **Weighted gradient flow for $\boldsymbol{\Theta}$:** find $\boldsymbol{T}_k = \boldsymbol{n}_k \otimes \boldsymbol{t}_k + \boldsymbol{t}_k \otimes \boldsymbol{n}_k$ such that $\boldsymbol{t}_k$ is tangent to $\boldsymbol{n}_k$ and for all $\boldsymbol{v}$ tangent to $\boldsymbol{n}_k$ (Bartels, Raisch (2014))

$$\frac{1}{\tau}\int_\Omega s_k^2 \nabla \boldsymbol{t}_k : \nabla \boldsymbol{v} + \boldsymbol{t}_k \cdot \boldsymbol{v} + \delta_\Theta E_1^h[s_k, \boldsymbol{\Theta}_k + \boldsymbol{T}_k; \boldsymbol{V}] = 0 \quad \forall \boldsymbol{V} = \boldsymbol{n}_k \otimes \boldsymbol{v} + \boldsymbol{v} \otimes \boldsymbol{n}_k.$$

  - **Projection:** update $\boldsymbol{\Theta}$ by

$$\boldsymbol{\Theta}_{k+1} := \frac{\boldsymbol{n}_k + \boldsymbol{t}_k}{|\boldsymbol{n}_k + \boldsymbol{t}_k|} \otimes \frac{\boldsymbol{n}_k + \boldsymbol{t}_k}{|\boldsymbol{n}_k + \boldsymbol{t}_k|}.$$

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

$$\frac{1}{2\tau}\int_\Omega |s_{k+1} - s_k|^2 + \delta_s E_1^h[s_{k+1}, \boldsymbol{\Theta}_{k+1}; z] + \underbrace{\delta_s E_2^h[s_{k+1}; z]}_{\text{convex splitting}} = 0 \quad \forall z,$$

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

- **Relaxation:** the effect of weight s_k^2 is to allow for larger variations of $\boldsymbol{t}_k$.

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Energy Decrease Property for the Q-Model

- **Variations in line field:** avoid nonlinear term $\boldsymbol{t} \otimes \boldsymbol{t}$ (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

$$E_1^h[s_N, \boldsymbol{\Theta}_N] + \frac{2}{\tau} \sum_{k=0}^{N-1} \left(\|s_k \nabla \boldsymbol{t}_k\|^2_{L^2(\Omega)} + \|\boldsymbol{t}_k\|^2_{L^2(\Omega)} + \|s_{k+1} - s_k\|^2 \right)$$
$$\leq E_1^h[s_0, \boldsymbol{\Theta}_0] \quad \forall N \geq 1.$$

Thus, the algorithm stops in a finite number of steps for any tolerance ε.

Why do we have a CFL condition?

- **Tangential variations:** In Step 1 we update $\Theta_k = I_h(\mathbf{n}_k \otimes \mathbf{n}_k)$ according to

$$\Theta_k + \mathbf{T}_k, \quad \boldsymbol{T}_k = \mathbf{n}_k \otimes \mathbf{t}_k + \mathbf{t}_k \otimes \mathbf{n}_k$$

with $\mathbf{t}_k(x_i) \cdot \mathbf{n}_k(x_i) = 0$ (nodal tangential update).

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

$$\big(\mathbf{n}_k + \mathbf{t}_k\big) \otimes \big(\mathbf{t}_k + \mathbf{n}_k\big) = \Theta_k + \mathbf{T}_k + \mathbf{t}_k \otimes \mathbf{t}_k$$

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

- **Correction term:** We must thus accound for $\mathbf{t}_k \otimes \mathbf{t}_k$

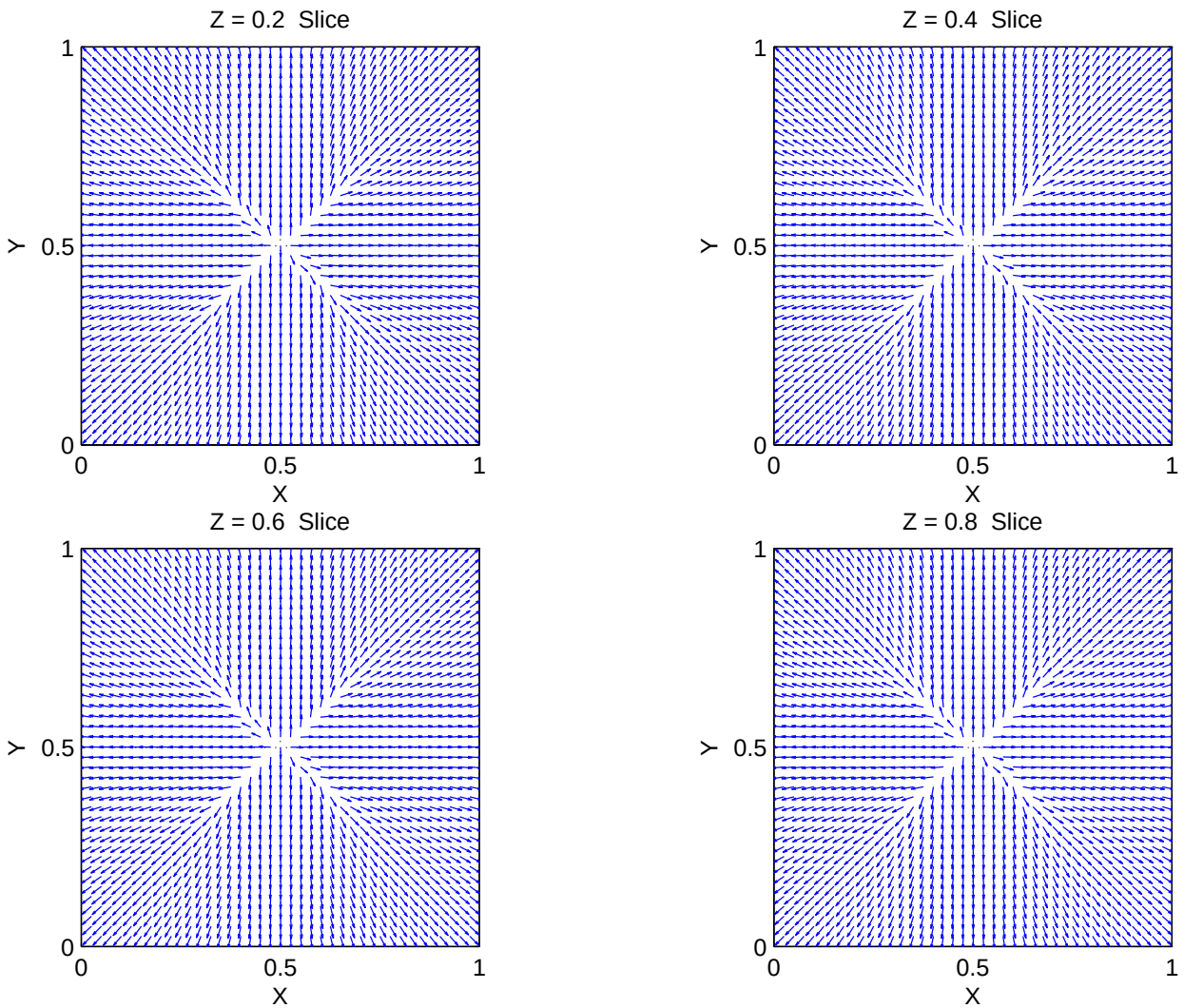
$$\sum_{i,j} k_{ij} \Big(s_k(x_i)^2 + s_k(x_j)^2 \Big) \big| \delta_{ij} (\mathbf{t}_k \otimes \mathbf{t}_k) \big|^2 \approx h^{-d} \Big(\int_\Omega s_k^2 |\nabla \mathbf{t}_k|^2 + |\mathbf{t}_k|^2 \Big)^2 .$$

An induction argument together with $\tau \leq C_0 h^{d/2}$, with C_0 proportional to $E_h[s_0, \boldsymbol{\Theta}_0]$, allows for control of this term.

Outline

Ericksen's Model: "Propeller" Defect $\kappa = 0.1$

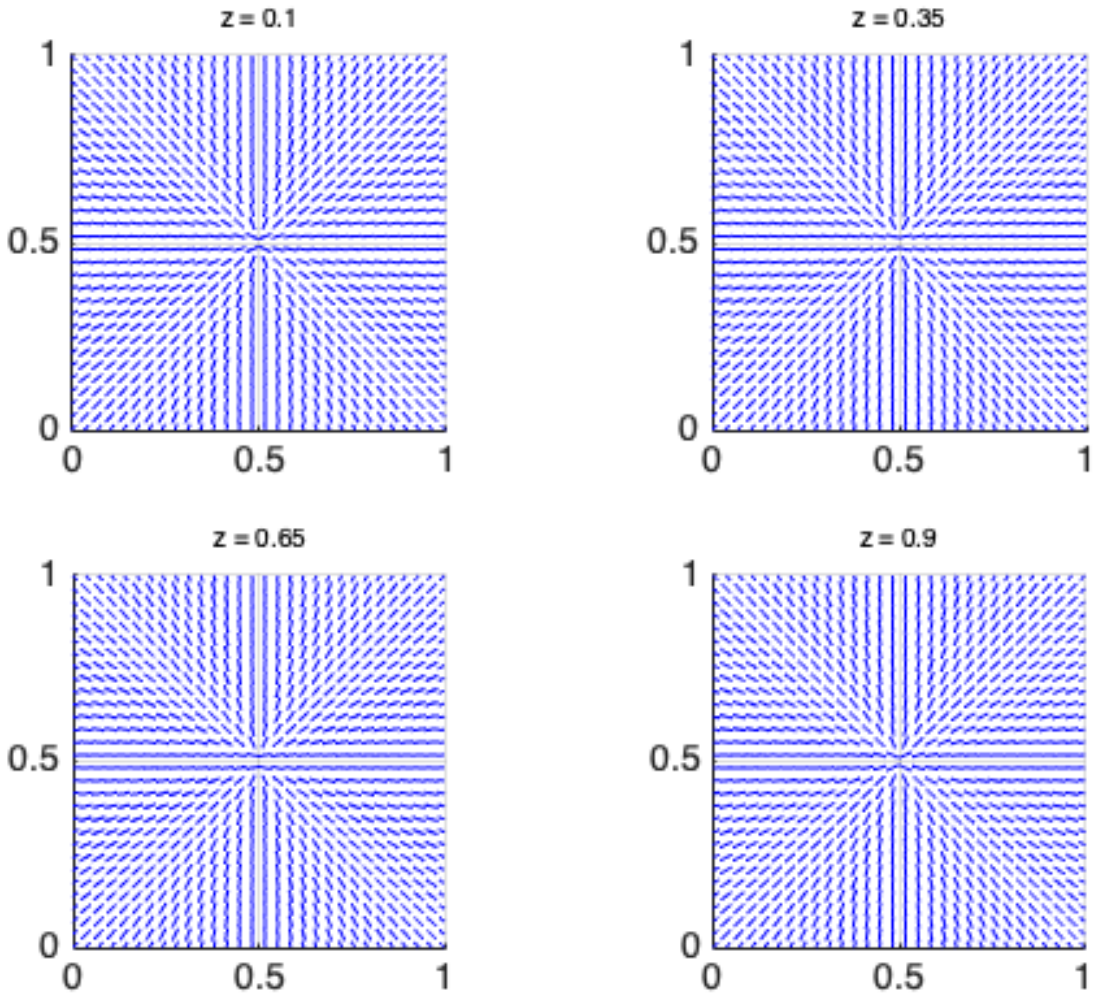
- **Director field at 4 slices:** $z = 0.2, 0.4, 0.6, 0.8$



- **Movie:** Director field at $z = 0$ **Movie:** 3d defect is marked in red.

Q-Model: 3-D Line Defect of Degree 1

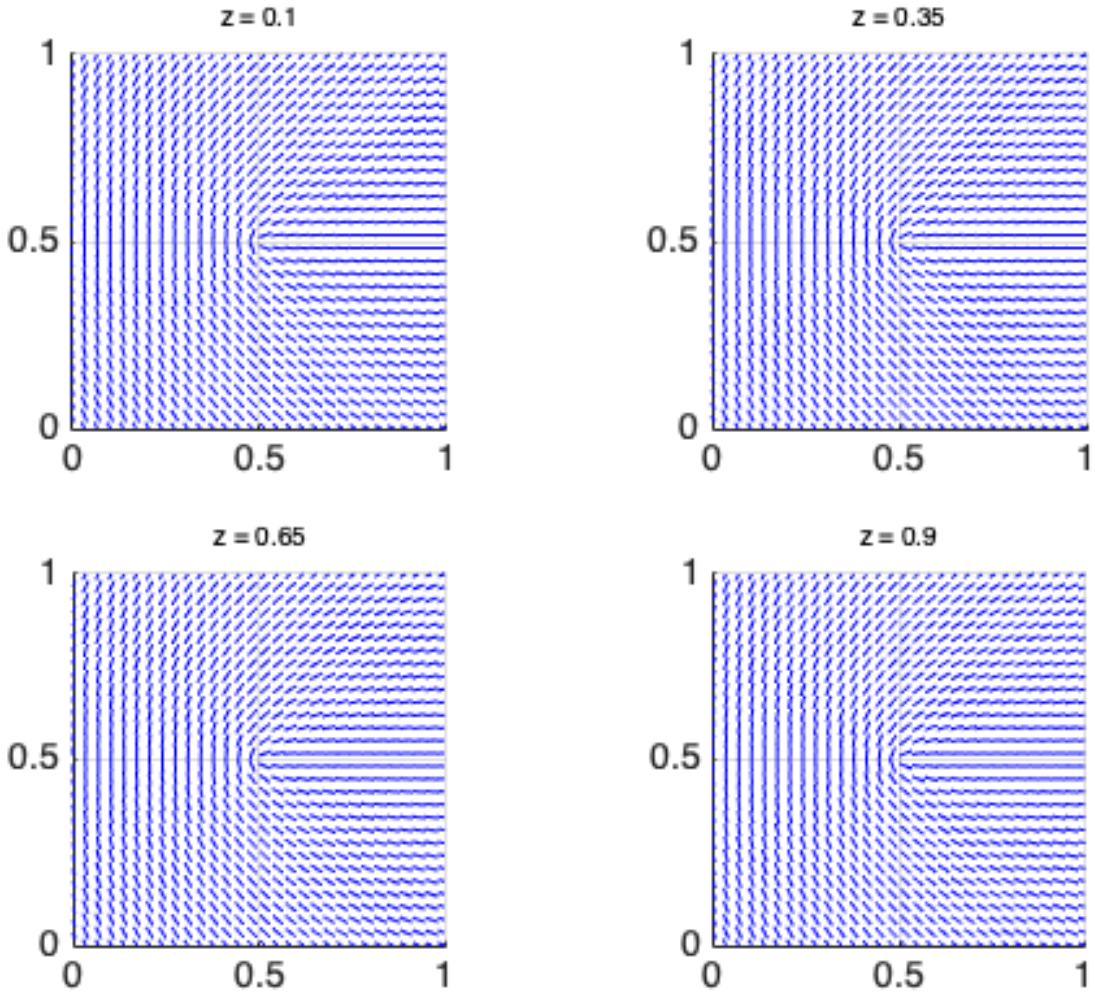
- **Line field at 4 slices:** $z = 0.1, 0.35, 0.65, 0.9$; $s_{\min} = 1.0 \times 10^{-2}$.



- **Movie:** Line field at $z = 0.5$. Gradient flow starts with line defect of degree 1 located at $(0.25, 025)$.

Q-Model: 3-D Line Defect of Degree $1/2$

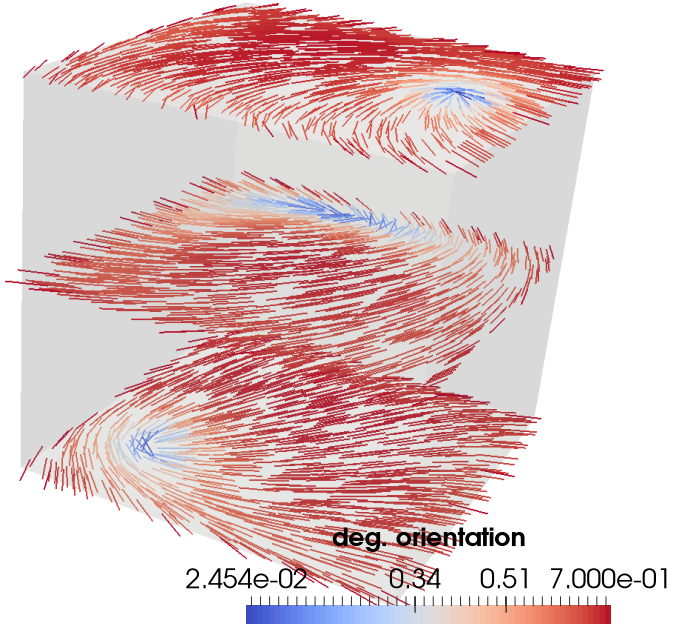
- **Line field at 4 slices:** $z = 0.1, 0.35, 0.65, 0.9$; $s_{\min} = 6.8 \times 10^{-2}$.

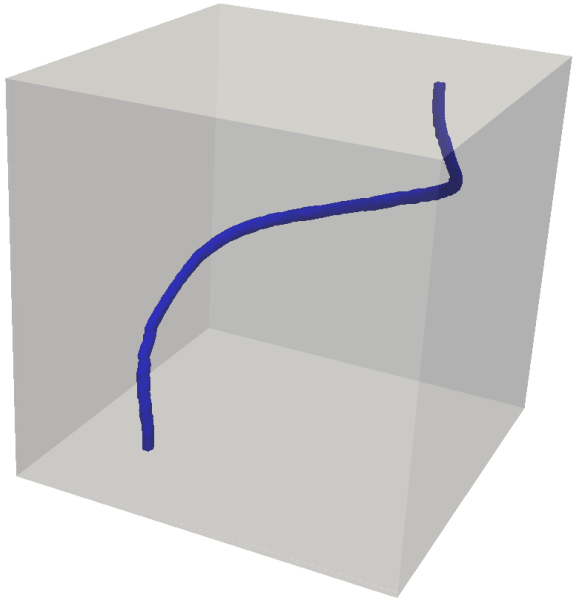


- **Movie:** Line field at $z = 0.5$. Gradient flow starts with line defect of degree 1 at $(0.25, 025)$.

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.

Outline

Electric Field Effect with Q-Model: Freedericksz Transition

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

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

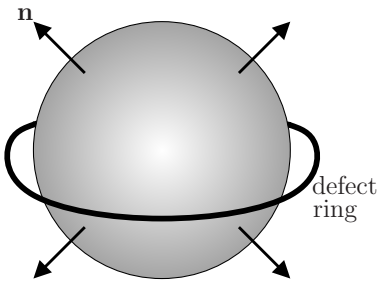
  Above, K_{ext} is a weight parameter, and $\overline{\varepsilon}, \gamma_a, \varepsilon_a$ are material constants.

- **Simulation:** Freedericksz transition with Dirichlet boundary conditions on the left and right of Ω and zero Neumann condition on top and bottom of Ω. The electric field is $\boldsymbol{E} = (1, 0)^\top$.

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 $(s, \mathbf{\Theta}) = (s_*, \boldsymbol{\nu} \otimes \boldsymbol{\nu})$ on colloidal surface with unit normal $\boldsymbol{\nu}$

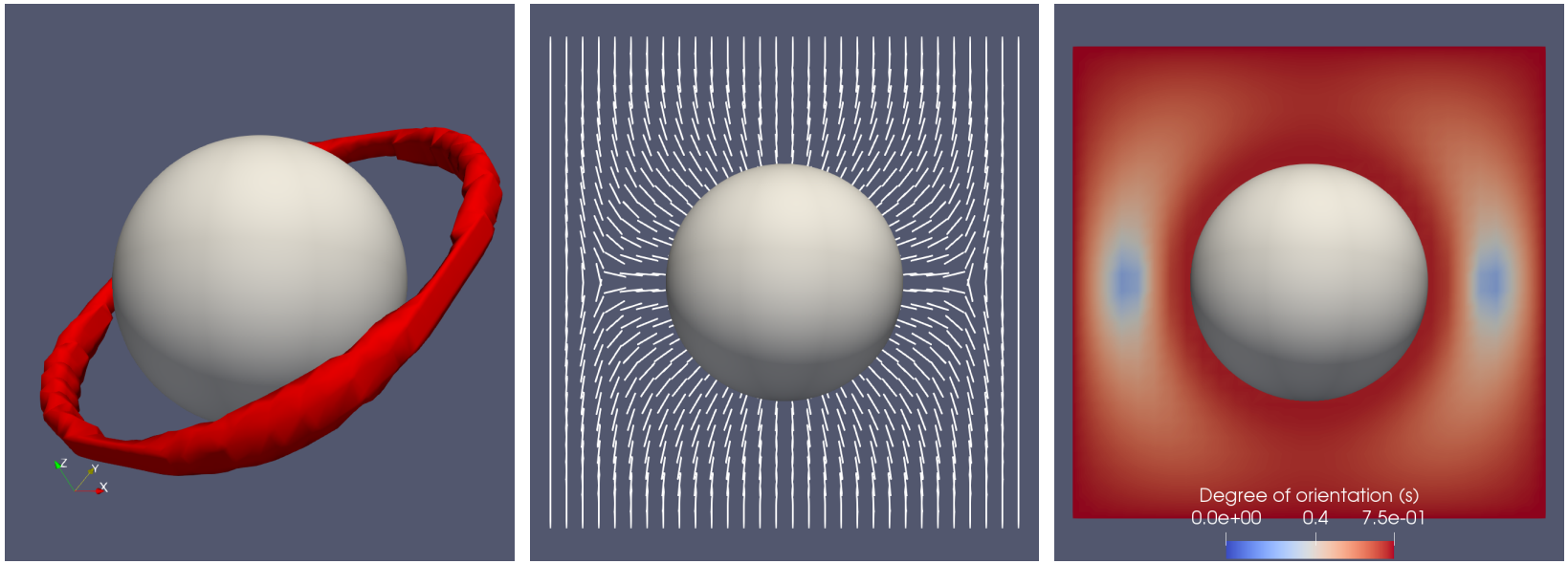
$$E_a[s, \mathbf{\Theta}] = \frac{K_a}{2} C_0 \epsilon \left(\int_\Omega s^2 \left(|\mathbf{\Theta}|^2 |\nabla \phi|^2 - \mathbf{\Theta} \nabla \phi \cdot \nabla \phi \right) + \int_\Omega |\nabla \phi|^2 (s - s^*) \right).$$

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

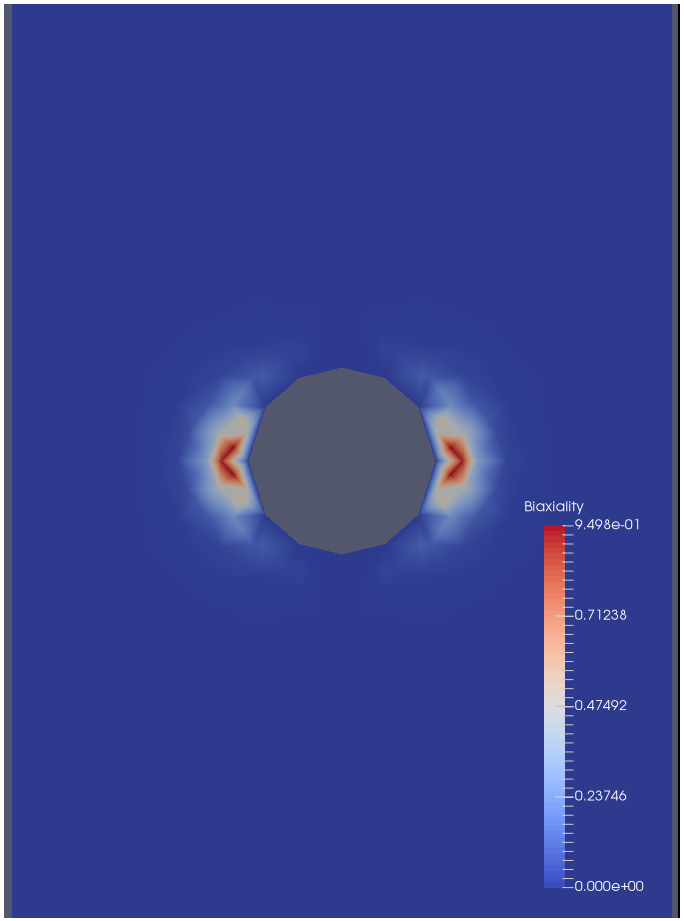


Left: isosurface $\{s = 0.2\}$. **Center:** line field slice at plane $\{y = 0.5\}$.
Right: degree of orientation slice at plane $\{y = 0.5\}$.

- **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)

$$0 \le \beta(\boldsymbol{Q}) = 1 - 6\frac{\left(\mathrm{tr}\boldsymbol{Q}^3\right)^2}{\left(\mathrm{tr}\boldsymbol{Q}^2\right)^3} \le 1 \quad \Rightarrow \quad \begin{cases} \beta(\boldsymbol{Q}) = 0 & \text{uniaxial} \\ \beta(\boldsymbol{Q}) = 1 & \text{biaxial} \end{cases}$$



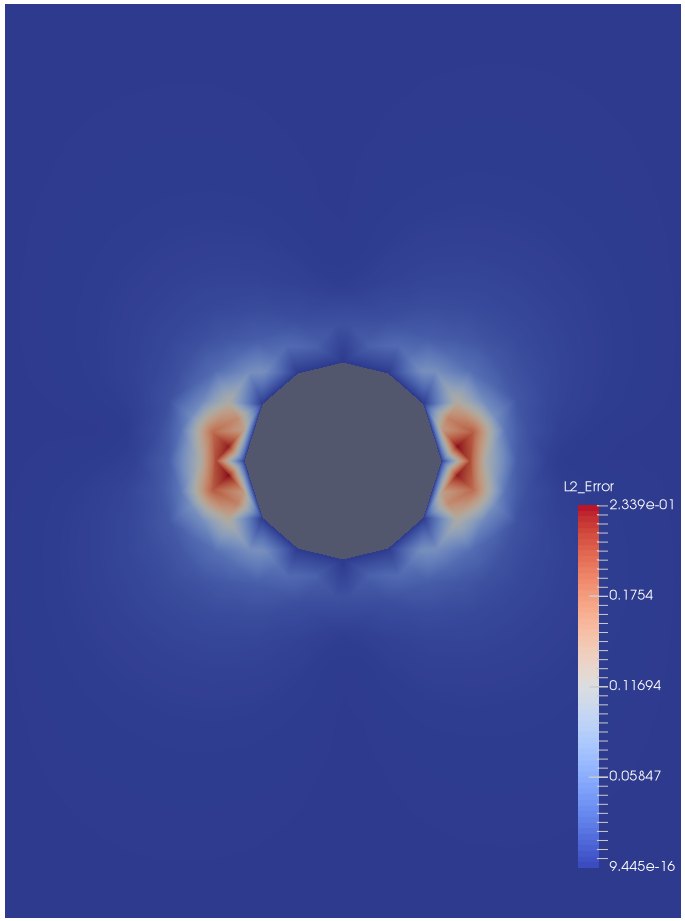


Figure (a): Measure of biaxiality $\beta(\boldsymbol{Q})$ (blue (uniaxial), red (biaxial));
Figure (b): plot of the function $|\boldsymbol{Q}_{\mathrm{LdG}} - \boldsymbol{Q}_{\mathrm{uni}}|$ (the error can be up to 15-20%).

Outline

Conclusions

- Structure preserving FEMs for the one constant Ericksen's model

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

  and the Landau-DeGennes Q-tensor model ($Q = s\boldsymbol{n}\otimes\boldsymbol{n}$)

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

- Γ-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.
- Γ-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:

- N, S.W. Walker, and W. Zhang, *A finite element method for nematic liquid crystals with variable degree of orientation*, SIAM J. Numer. Anal. 55, 3 (2017), 1357-1386.
- N, S.W. Walker, and W. Zhang, *The Ericksen model of liquid crystals with colloidal and electric effects*, J. Comp. Phys. 352 (2018), 568–601.
- J.P. Borthagaray, N, and S.W. Walker, *A structure preserving FEM for the Q-model of uniaxial nematic liquid crystals*, (submitted).