A Finite Element Method For Nematic Liquid Crystals With Variable Degree Of Orientation

Shawn W. Walker

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

joint with

Ricardo H. Nochetto, University of Maryland

Wujun Zhang, University of Maryland

Complex Materials:
Mathematical Models and Numerical Methods
University of Oslo, June 11, 2015

Outline

OUTLINE

Macroscopic Model of Liquid Crystals (De Gennes)

- Liquid crystals find everyday use in modern technology.
- LCDs, optics, etc.

- Liquid crystal *molecules* are often *idealized* as elongated rods or ellipsoidal disks.
- Further simplify by an averaging procedure to replace local arrangements of many rods by a **few** *order parameters*.

Essentially, the **state** of the system is:

- The local (average) orientation of molecules.
- The local (average) degree of orientation.

One model that captures this is the Q-tensor approach [De Gennes 74].

Macroscopic Model of Liquid Crystals (De Gennes)

- Liquid crystals find everyday use in modern technology.
- LCDs, optics, etc.

- Liquid crystal *molecules* are often *idealized* as elongated rods or ellipsoidal disks.
- Further simplify by an averaging procedure to replace local arrangements of many rods by a **few** *order parameters*.

Essentially, the **state** of the system is:

- The local (average) orientation of molecules.
- The local (average) degree of orientation.

One model that captures this is the $\boldsymbol{Q}$-tensor approach [De Gennes 74].

Model: Ericksen's model

- $\boldsymbol{Q}$ tensor is a symmetric, traceless 3×3 tensor. Thus, $\boldsymbol{Q}$ is of the form

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

  with eigenvalues between $-1/3$ and $2/3$.
- Uniaxial liquid crystal: $\boldsymbol{Q}$ tensor reduces to $\boldsymbol{Q} = s(\boldsymbol{n} \otimes \boldsymbol{n} - \frac{1}{3}I)$.
- Further simplification: deal with the director $\boldsymbol{n}$.
- The equilibrium state minimizes (one-constant Ericksen's model):

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

  where $\kappa > 0$ and ψ_B is a double well potential.
- 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:

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

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

Model: Ericksen's model

- $\boldsymbol{Q}$ tensor is a symmetric, traceless 3×3 tensor. Thus, $\boldsymbol{Q}$ is of the form

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

  with eigenvalues between $-1/3$ and $2/3$.
- Uniaxial liquid crystal: $\boldsymbol{Q}$ tensor reduces to $\boldsymbol{Q} = s(\boldsymbol{n} \otimes \boldsymbol{n} - \frac{1}{3}I)$.
- Further simplification: deal with the director $\boldsymbol{n}$.
- The equilibrium state minimizes (one-constant Ericksen's model):

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

  where $\kappa > 0$ and ψ_B is a double well potential.
- 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:

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

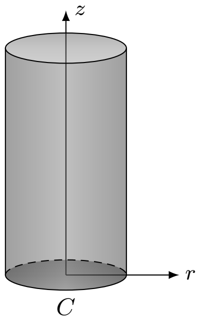
- $s = -1/2$: perpendicular to $\boldsymbol{n}$.

Ericksen's model vs. Oseen-Frank model

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

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

- Line and plane defects have **infinite** energy in the Oseen-Frank model:



- Line defects:

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

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

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

- Ericksen's model regularizes the defect.
- Goal: design a robust finite element method to capture these defects.

Literature Review

Hardt Kinderlehrer Lin (1986), Kinderlehrer (1991), Kinderlehrer, Ou, Walkington (1993)
Brezis (1987, 1989) Ericksen (1991)
book: Virga (1994)
Ambrosio (1990)
Lin (1989, 1991), Lin Liu (1995)
Bauman Calderer Liu Phillips (2002), Bauman Park Phillps (2012)
Ball Zarnescu (2011)

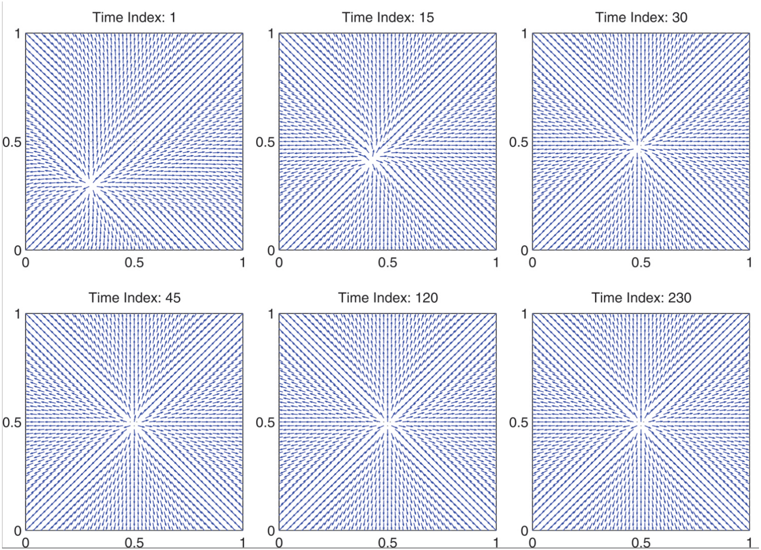
Alouges (1997)
Badia Guillén-González Gutiérrez-Santacreu (2011, 2013)
Bartels (2010)
Cohen Lin Luskin (1989)
Liu Walkington (2000)
Yang Forest Li Liu Shen Wang (2013)

Calderer, Golovaty, Lin, Liu (2002) (Time evolution for Ericksen 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)

OUTLINE

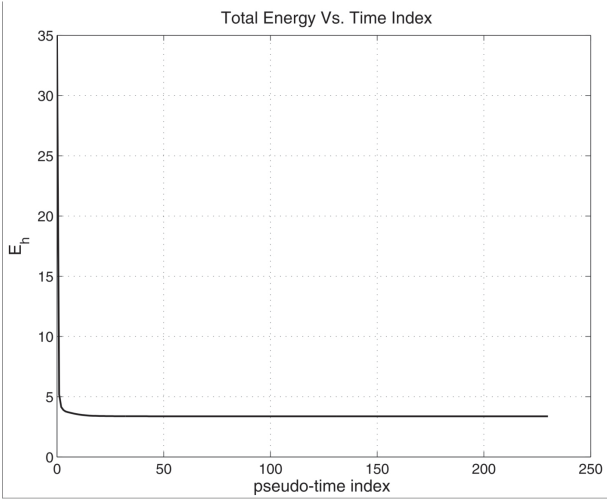
Numerical Experiments: (point defect in $2d$)

Consider the Dirichlet boundary conditions $s = s^*, \quad \boldsymbol{n} = \frac{\boldsymbol{x}}{|\boldsymbol{x}|}$. MOVIE



Numerical Experiments: (point defect in $2d$)

Energy Decrease:



Admissible class

- Assume $\kappa > 0$. We seek a **discrete energy** E_1^h to approximate

$$E_1 := \int_\Omega \kappa |\nabla s|^2 + s^2 |\nabla \boldsymbol{n}|^2 dx.$$

- Since $\nabla |\boldsymbol{n}|^2 = 2(\nabla \boldsymbol{n})\boldsymbol{n} = \mathbf{0}$, we have an **identity**:

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

  We rewrite the energy [Ambrosio 90, Lin 91]:

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

  i.e. a simple quadratic functional, but with a **negative** term.

- Admissible class:

$$\mathcal{A} := \{(s, \boldsymbol{n}) : s \in H^1(\Omega),\ \boldsymbol{u} = s\boldsymbol{n} \in H^1(\Omega) \text{ and } |\boldsymbol{n}| = 1 \text{ a.e. in } \Omega\}.$$

Numerical Discretization

- Let $\mathcal{T}_h = \{T\}$ be a conforming, shape-regular triangulation of Ω, with set of nodes (vertices) denoted by $\mathcal{N}_h$.
- Exact solution: $(s, \boldsymbol{n})$; Discrete solution $(S, \boldsymbol{N})$ or $(s_h, \boldsymbol{n}_h)$.
- Piecewise linear approximation: $S \in W_h$, $\boldsymbol{N} \in V_h$:

$$
\begin{aligned}
W_h &:= \{S \in H^1(\Omega) : S|_T \text{ is affine}\}, \\
U_h &:= \{\boldsymbol{U} \in H^1(\Omega)^d : \boldsymbol{U}|_T \text{ is affine in each component}\}, \\
V_h &:= \{\boldsymbol{N} \in U_h : |\boldsymbol{N}(x_i)| = 1 \text{ at all nodes } x_i \in \mathcal{N}_h\}.
\end{aligned}
$$

- I.e. impose the unit length constraint at the mesh nodes.
- Denote the continuous piecewise linear "hat" basis functions by $\{\phi_i\}$.
- 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, then this condition is true.

Numerical Discretization

- Let $\mathcal{T}_h = \{T\}$ be a conforming, shape-regular triangulation of Ω, with set of nodes (vertices) denoted by $\mathcal{N}_h$.
- Exact solution: $(s, \boldsymbol{n})$; Discrete solution $(S, \boldsymbol{N})$ or $(s_h, \boldsymbol{n}_h)$.
- Piecewise linear approximation: $S \in W_h$, $\boldsymbol{N} \in V_h$:

$$
\begin{aligned}
W_h &:= \{S \in H^1(\Omega) : S|_T \text{ is affine}\}, \\
U_h &:= \{\boldsymbol{U} \in H^1(\Omega)^d : \boldsymbol{U}|_T \text{ is affine in each component}\}, \\
V_h &:= \{\boldsymbol{N} \in U_h : |\boldsymbol{N}(x_i)| = 1 \text{ at all nodes } x_i \in \mathcal{N}_h\}.
\end{aligned}
$$

- I.e. impose the unit length constraint at the mesh nodes.
- Denote the continuous piecewise linear "hat" basis functions by $\{\phi_i\}$.
- 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, then this condition is true.

Discretization of the Energy

- The condition $|\boldsymbol{N}(x)| = 1$ is *only at the nodes* $x = x_i$,
- This suggests to view the **discrete energy** in terms of **nodal values**.
- For a piecewise linear function S, we have

$$\int_\Omega |\nabla S|^2 dx = \frac{1}{2} \sum_{i,j} k_{ij} (S_i - S_j)^2,$$

where $S_i = S(x_i)$ for all nodes x_i.

- We approximate

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

by a **discrete energy:**

$$E_1^h := \underbrace{\frac{\kappa}{2} \sum_{i,j=1}^{N} k_{ij} \left(S_i - S_j\right)^2}_{\text{standard}} + \underbrace{\frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left(\frac{S_i^2 + S_j^2}{2}\right) |\boldsymbol{N}_i - \boldsymbol{N}_j|^2}_{\textbf{not}\text{ standard}},$$

where $\boldsymbol{N}_i = \boldsymbol{N}(x_i)$ for all nodes x_i.

Discretization of the Energy

- The condition $|\boldsymbol{N}(x)| = 1$ is *only at the nodes* $x = x_i$,
- This suggests to view the **discrete energy** in terms of **nodal values**.
- For a piecewise linear function S, we have

$$\int_\Omega |\nabla S|^2 dx = \frac{1}{2} \sum_{i,j} k_{ij} (S_i - S_j)^2,$$

  where $S_i = S(x_i)$ for all nodes x_i.
- We approximate

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

  by a **discrete energy:**

$$E_1^h := \underbrace{\frac{\kappa}{2} \sum_{i,j=1}^{N} k_{ij} \left(S_i - S_j\right)^2}_{\text{standard}} + \underbrace{\frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left(\frac{S_i^2 + S_j^2}{2}\right) |\boldsymbol{N}_i - \boldsymbol{N}_j|^2}_{\textbf{not}\text{ standard}},$$

  where $\boldsymbol{N}_i = \boldsymbol{N}(x_i)$ for all nodes x_i.

Stability of the Discrete Energy

- Let $\boldsymbol{U} \in U_h$ such that $\boldsymbol{U}(x_i) = S(x_i)\boldsymbol{N}(x_i)$ for all nodes x_i.
- Energy inequality:

$$E_1^h[\Omega, S, \boldsymbol{N}] \geq (\kappa - 1)\int_\Omega |\nabla S|^2 dx + \int_\Omega |\nabla \boldsymbol{U}|^2 dx.$$

- Moreover,

$$E_1^h[\Omega, S, \boldsymbol{N}] \geq (\kappa - 1)\int_\Omega |\nabla I_h|S||^2 dx + \int_\Omega |\nabla \widetilde{\boldsymbol{U}}|^2 dx.$$

- I_h is the linear interpolant of $|S|$.
- $\widetilde{\boldsymbol{U}} \in U_h$, such that $\widetilde{\boldsymbol{U}}(x_i) = |S(x_i)|\boldsymbol{N}(x_i)$ for all nodes x_i.

Remark: eventually, we need the right-hand-side to be **convex** with respect to the **gradient**. Thus, we need $|S|$.

Stability of the Discrete Energy

- Let $\boldsymbol{U} \in U_h$ such that $\boldsymbol{U}(x_i) = S(x_i)\boldsymbol{N}(x_i)$ for all nodes x_i.
- Energy inequality:

$$E_1^h[\Omega, S, \boldsymbol{N}] \geq (\kappa - 1)\int_\Omega |\nabla S|^2 dx + \int_\Omega |\nabla \boldsymbol{U}|^2 dx.$$

- Moreover,

$$E_1^h[\Omega, S, \boldsymbol{N}] \geq (\kappa - 1)\int_\Omega |\nabla I_h|S||^2 dx + \int_\Omega |\nabla \widetilde{\boldsymbol{U}}|^2 dx.$$

- I_h is the linear interpolant of $|S|$.
- $\widetilde{\boldsymbol{U}} \in U_h$, such that $\widetilde{\boldsymbol{U}}(x_i) = |S(x_i)|\boldsymbol{N}(x_i)$ for all nodes x_i.

Remark: eventually, we need the right-hand-side to be **convex** with respect to the **gradient**. Thus, we need $|S|$.

Stability of the Discrete Energy

prove this: $E_1^h \geq (\kappa - 1) \int_\Omega |\nabla S|^2 dx + \int_\Omega |\nabla \boldsymbol{U}|^2 dx.$

$$\int_\Omega |\nabla \boldsymbol{U}|^2 dx = \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} | \underbrace{S_i \boldsymbol{N}_i}_{\boldsymbol{U}_i} - \underbrace{S_j \boldsymbol{N}_j}_{\boldsymbol{U}_j} |^2$$

$$= \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left| \left(\frac{S_i + S_j}{2} \right) (\boldsymbol{N}_i - \boldsymbol{N}_j) + (S_i - S_j) \left(\frac{\boldsymbol{N}_i + \boldsymbol{N}_j}{2} \right) \right|^2.$$

The unit length constraint on $\boldsymbol{N}$ at the nodes implies: $(\boldsymbol{N}_i - \boldsymbol{N}_j) \cdot (\boldsymbol{N}_i + \boldsymbol{N}_j) = |\boldsymbol{N}_i|^2 - |\boldsymbol{N}_j|^2 = 0$. Thus,

$$\int_\Omega |\nabla \boldsymbol{U}|^2 dx = \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left(\frac{S_i + S_j}{2} \right)^2 |\boldsymbol{N}_i - \boldsymbol{N}_j|^2 + \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} (S_i - S_j)^2 \left| \frac{\boldsymbol{N}_i + \boldsymbol{N}_j}{2} \right|^2$$

$$= \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left(\frac{S_i + S_j}{2} \right)^2 |\boldsymbol{N}_i - \boldsymbol{N}_j|^2 + \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} (S_i - S_j)^2 - \frac{1}{2} \mathcal{E},$$

where we used $\left| \frac{\boldsymbol{N}_i + \boldsymbol{N}_j}{2} \right|^2 = 1 - \left| \frac{\boldsymbol{N}_i - \boldsymbol{N}_j}{2} \right|^2$.

Stability of the Discrete Energy

$$\textbf{prove this:} \quad E_1^h \geq (\kappa - 1) \int_\Omega |\nabla S|^2 dx + \int_\Omega |\nabla \boldsymbol{U}|^2 dx.$$

$$\int_\Omega |\nabla \boldsymbol{U}|^2 dx = \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} |\underbrace{S_i \boldsymbol{N}_i}_{\boldsymbol{U}_i} - \underbrace{S_j \boldsymbol{N}_j}_{\boldsymbol{U}_j}|^2$$

$$= \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left| \left(\frac{S_i + S_j}{2} \right) (\boldsymbol{N}_i - \boldsymbol{N}_j) + (S_i - S_j) \left(\frac{\boldsymbol{N}_i + \boldsymbol{N}_j}{2} \right) \right|^2 .$$

The unit length constraint on $\boldsymbol{N}$ at the nodes implies:
$(\boldsymbol{N}_i - \boldsymbol{N}_j) \cdot (\boldsymbol{N}_i + \boldsymbol{N}_j) = |\boldsymbol{N}_i|^2 - |\boldsymbol{N}_j|^2 = 0$. Thus,

$$\int_\Omega |\nabla \boldsymbol{U}|^2 dx = \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left(\frac{S_i + S_j}{2} \right)^2 |\boldsymbol{N}_i - \boldsymbol{N}_j|^2 + \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} (S_i - S_j)^2 \left| \frac{\boldsymbol{N}_i + \boldsymbol{N}_j}{2} \right|^2$$

$$= \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left(\frac{S_i + S_j}{2} \right)^2 |\boldsymbol{N}_i - \boldsymbol{N}_j|^2 + \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} (S_i - S_j)^2 - \frac{1}{2} \mathcal{E},$$

where we used $\left| \frac{\boldsymbol{N}_i + \boldsymbol{N}_j}{2} \right|^2 = 1 - \left| \frac{\boldsymbol{N}_i - \boldsymbol{N}_j}{2} \right|^2$.

Stability of the Discrete Energy

prove this: $E_1^h \geq (\kappa - 1) \int_\Omega |\nabla S|^2 dx + \int_\Omega |\nabla \boldsymbol{U}|^2 dx.$

$$\int_\Omega |\nabla \boldsymbol{U}|^2 dx = \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} | \underbrace{S_i \boldsymbol{N}_i}_{\boldsymbol{U}_i} - \underbrace{S_j \boldsymbol{N}_j}_{\boldsymbol{U}_j} |^2$$

$$= \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left| \left(\frac{S_i + S_j}{2} \right) (\boldsymbol{N}_i - \boldsymbol{N}_j) + (S_i - S_j) \left(\frac{\boldsymbol{N}_i + \boldsymbol{N}_j}{2} \right) \right|^2.$$

The unit length constraint on $\boldsymbol{N}$ at the nodes implies:
$(\boldsymbol{N}_i - \boldsymbol{N}_j) \cdot (\boldsymbol{N}_i + \boldsymbol{N}_j) = |\boldsymbol{N}_i|^2 - |\boldsymbol{N}_j|^2 = 0$. Thus,

$$\int_\Omega |\nabla \boldsymbol{U}|^2 dx = \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left(\frac{S_i + S_j}{2} \right)^2 |\boldsymbol{N}_i - \boldsymbol{N}_j|^2 + \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} (S_i - S_j)^2 \left| \frac{\boldsymbol{N}_i + \boldsymbol{N}_j}{2} \right|^2$$

$$= \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left(\frac{S_i + S_j}{2} \right)^2 |\boldsymbol{N}_i - \boldsymbol{N}_j|^2 + \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} (S_i - S_j)^2 - \frac{1}{2} \mathcal{E},$$

where we used $\left| \frac{\boldsymbol{N}_i + \boldsymbol{N}_j}{2} \right|^2 = 1 - \left| \frac{\boldsymbol{N}_i - \boldsymbol{N}_j}{2} \right|^2$.

Stability of the Discrete Energy

$$\int_\Omega |\nabla \boldsymbol{U}|^2 dx = \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} (S_i - S_j)^2 + \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left(\frac{S_i + S_j}{2} \right)^2 |\boldsymbol{N}_i - \boldsymbol{N}_j|^2 - \frac{1}{2} \mathcal{E},$$

where

$$\mathcal{E} := \sum_{i,j=1}^{N} k_{ij} \left(S_i - S_j\right)^2 \left| \frac{\boldsymbol{N}_i - \boldsymbol{N}_j}{2} \right|^2 \qquad \text{(positive term).}$$

Next, plug in:

$$\left(\frac{S_i + S_j}{2} \right)^2 = \left(\frac{S_i^2 + S_j^2}{2} \right) - \left(\frac{S_i - S_j}{2} \right)^2,$$

to get

$$\int_\Omega |\nabla \boldsymbol{U}|^2 dx = \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} (S_i - S_j)^2 + \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left(\frac{S_i^2 + S_j^2}{2} \right) |\boldsymbol{N}_i - \boldsymbol{N}_j|^2 - \mathcal{E},$$

Stability of the Discrete Energy

$$\int_\Omega |\nabla \boldsymbol{U}|^2 dx = \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} (S_i - S_j)^2 + \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left(\frac{S_i + S_j}{2} \right)^2 |\boldsymbol{N}_i - \boldsymbol{N}_j|^2 - \frac{1}{2} \mathcal{E},$$

where

$$\mathcal{E} := \sum_{i,j=1}^{N} k_{ij} \left(S_i - S_j\right)^2 \left| \frac{\boldsymbol{N}_i - \boldsymbol{N}_j}{2} \right|^2 \qquad \text{(positive term).}$$

Next, plug in:

$$\left(\frac{S_i + S_j}{2} \right)^2 = \left(\frac{S_i^2 + S_j^2}{2} \right) - \left(\frac{S_i - S_j}{2} \right)^2,$$

to get

$$\int_\Omega |\nabla \boldsymbol{U}|^2 dx = \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} (S_i - S_j)^2 + \frac{1}{2} \sum_{i,j=1}^{N} k_{ij} \left(\frac{S_i^2 + S_j^2}{2} \right) |\boldsymbol{N}_i - \boldsymbol{N}_j|^2 - \mathcal{E},$$

Stability of the Discrete Energy

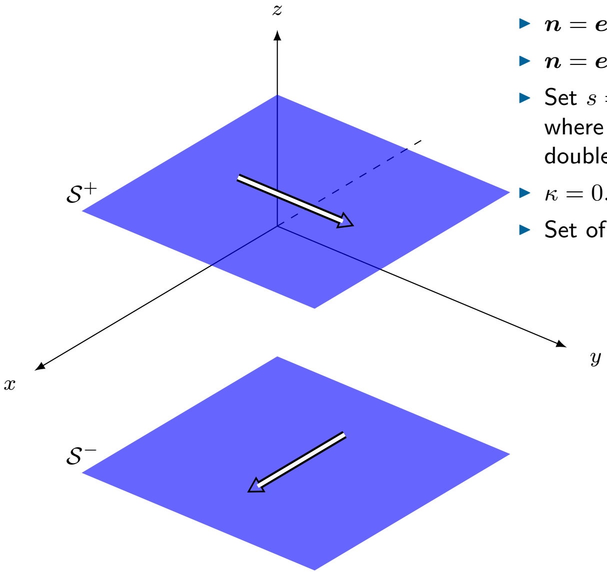
prove this: $E_1^h \geq (\kappa - 1)\int_\Omega |\nabla S|^2 dx + \int_\Omega |\nabla \boldsymbol{U}|^2 dx.$

Adding $(\kappa - 1)\int_\Omega |\nabla S|^2 dx$ to both sides gives

$$
\begin{aligned}
&(\kappa - 1)\int_\Omega |\nabla S|^2 dx + \int_\Omega |\nabla \boldsymbol{U}|^2 dx \\
&= \frac{\kappa}{2}\sum_{i,j=1}^{N} k_{ij}(S_i - S_j)^2 + \frac{1}{2}\sum_{i,j=1}^{N} k_{ij}\left(\frac{S_i^2 + S_j^2}{2}\right)|\boldsymbol{N}_i - \boldsymbol{N}_j|^2 - \mathcal{E} \\
&\leq E_1^h.
\end{aligned}
$$

Note that $\mathcal{E} \geq 0$ provided the meshes are weakly acute.

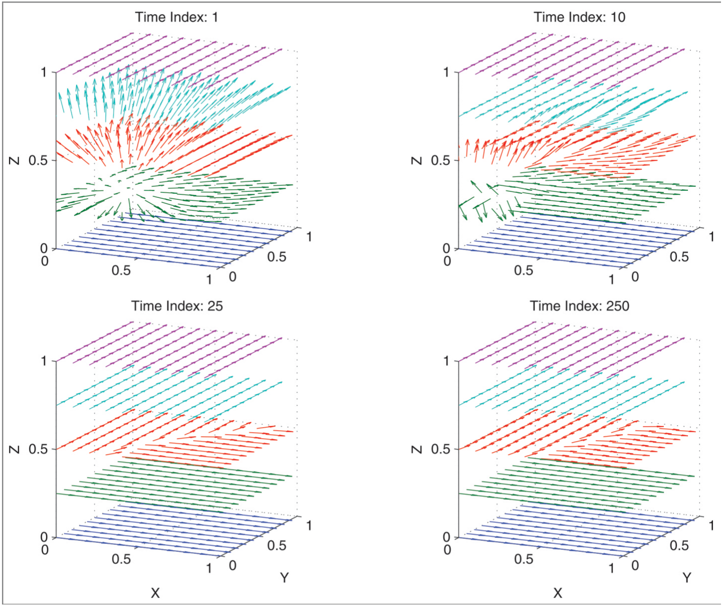
Numerical Experiments: (plane defect in $3d$) [Ambrosio Virga 1991]



- $\boldsymbol{n} = \boldsymbol{e}_1$ on $\mathcal{S}^-$.
- $\boldsymbol{n} = \boldsymbol{e}_2$ on $\mathcal{S}^+$.
- Set $s = s_0$ on $\mathcal{S}^+$ and $\mathcal{S}^-$, where s_0 is the minimizer of double well potential ψ_B.
- $\kappa = 0.2$
- Set of defect: $\{z = 1/2\}$.

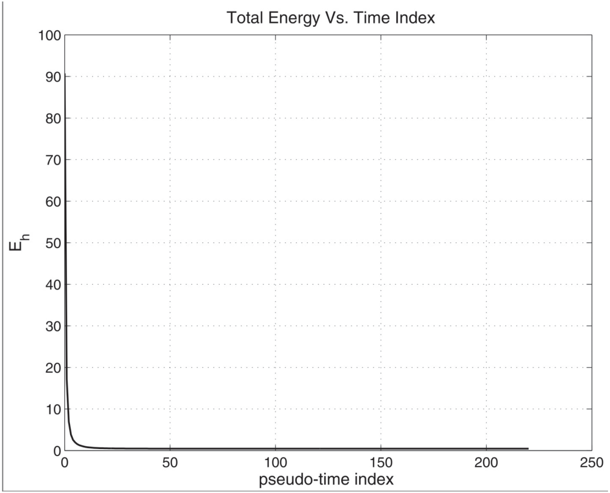
Numerical Experiments: (plane defect in $3d$)

MOVIE



Numerical Experiments: (plane defect in $3d$)

Energy Decrease:



OUTLINE

Main Theorem

Γ-Convergence of the Discrete Energy E_1^h:

- Let $\{\mathcal{T}_h\}$ be a sequence of weakly acute meshes.
- **lim-sup:** there exists a sequence $\{(s_h, \boldsymbol{n}_h)\}$, such that $(s_h, \boldsymbol{n}_h)$ converges to $(s, \boldsymbol{n})$ in L^2, and

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

- **lim-inf:** for *every* sequence $\{(s_h, \boldsymbol{n}_h)\}$, such that $(s_h, \boldsymbol{n}_h)$ converges to $(s, \boldsymbol{n})$ in L^2, we have

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

Convergence of the Finite Element Method:

- $E_1^h[s_h, \boldsymbol{n}_h]$ is coercive: any sequence $\{(s_h, \boldsymbol{n}_h)\}$ with finite discrete energy is pre-compact in L^2.
- Let $\{(s_h, \boldsymbol{n}_h)\}$ be a minimizing sequence of $E_1^h[s_h, \boldsymbol{n}_h]$.
- Then $(s_h, \boldsymbol{n}_h)$ converges to $(s, \boldsymbol{n})$ in L^2, where $(s, \boldsymbol{n})$ is a minimizer of $E_1[s, \boldsymbol{n}]$.

Main Theorem

Γ-Convergence of the Discrete Energy E_1^h:

- Let $\{\mathcal{T}_h\}$ be a sequence of weakly acute meshes.
- **lim-sup:** there exists a sequence $\{(s_h, \boldsymbol{n}_h)\}$, such that $(s_h, \boldsymbol{n}_h)$ converges to $(s, \boldsymbol{n})$ in L^2, and

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

- **lim-inf:** for *every* sequence $\{(s_h, \boldsymbol{n}_h)\}$, such that $(s_h, \boldsymbol{n}_h)$ converges to $(s, \boldsymbol{n})$ in L^2, we have

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

Convergence of the Finite Element Method:

- $E_1^h[s_h, \boldsymbol{n}_h]$ is coercive: any sequence $\{(s_h, \boldsymbol{n}_h)\}$ with finite discrete energy is pre-compact in L^2.
- Let $\{(s_h, \boldsymbol{n}_h)\}$ be a minimizing sequence of $E_1^h[s_h, \boldsymbol{n}_h]$.
- Then $(s_h, \boldsymbol{n}_h)$ converges to $(s, \boldsymbol{n})$ in L^2, where $(s, \boldsymbol{n})$ is a minimizer of $E_1[s, \boldsymbol{n}]$.

Limit-Sup Inequality

Let $(s, \boldsymbol{n})$ be in $\mathcal{A}$ and set $\boldsymbol{u} = s\boldsymbol{n}$. Then

$$E_1^h[s_h, \boldsymbol{n}_h] \to E_1[s, \boldsymbol{n}], \quad \text{as} \quad h \to 0,$$

where $(s_h, \boldsymbol{n}_h)$ are the Lagrange interpolants of $(s, \boldsymbol{n})$.

Proof:

- Recall the identity

$$E_1^h[s_h, \boldsymbol{n}_h] = (\kappa - 1) \int_\Omega |\nabla s_h|^2 dx + \int_\Omega |\nabla \boldsymbol{u}_h|^2 dx + \mathcal{E}$$

- Since $s_h \to s$, $\boldsymbol{u}_h \to \boldsymbol{u}$, we only need to show

$$\mathcal{E} = \sum_{i,j=1}^{N} k_{ij} \left(s_i - s_j\right)^2 \left|\frac{\boldsymbol{n}_i - \boldsymbol{n}_j}{2}\right|^2 \to 0, \quad \text{as} \quad h \to 0,$$

  where $s_i = s_h(x_i)$, $\boldsymbol{n}_i = \boldsymbol{n}_h(x_i)$.
- $\mathcal{E} \approx 2h^2 \int_\Omega |\nabla s_h|^2 dx$ if $\boldsymbol{n}$ is smooth.
- But $\boldsymbol{n}$ may have a **discontinuity**.

Limit-Sup Inequality

Let $(s, \boldsymbol{n})$ be in $\mathcal{A}$ and set $\boldsymbol{u} = s\boldsymbol{n}$. Then

$$E_1^h[s_h, \boldsymbol{n}_h] \to E_1[s, \boldsymbol{n}], \quad \text{as} \quad h \to 0,$$

where $(s_h, \boldsymbol{n}_h)$ are the Lagrange interpolants of $(s, \boldsymbol{n})$.

Proof:

- Recall the identity

$$E_1^h[s_h, \boldsymbol{n}_h] = (\kappa - 1) \int_\Omega |\nabla s_h|^2 dx + \int_\Omega |\nabla \boldsymbol{u}_h|^2 dx + \mathcal{E}$$

- Since $s_h \to s$, $\boldsymbol{u}_h \to \boldsymbol{u}$, we only need to show

$$\mathcal{E} = \sum_{i,j=1}^{N} k_{ij} \left(s_i - s_j\right)^2 \left| \frac{\boldsymbol{n}_i - \boldsymbol{n}_j}{2} \right|^2 \to 0, \quad \text{as} \quad h \to 0,$$

  where $s_i = s_h(x_i)$, $\boldsymbol{n}_i = \boldsymbol{n}_h(x_i)$.
- $\mathcal{E} \approx 2h^2 \int_\Omega |\nabla s_h|^2 dx$ if $\boldsymbol{n}$ is smooth.
- But $\boldsymbol{n}$ may have a **discontinuity**.

Consistency of the Discrete Energy

Proof:

We divide Ω into two regions:

$$\mathcal{S}_\epsilon = \{x \in \Omega, \ |s(x)| < \epsilon\} \quad \text{and} \quad \mathcal{K}_\epsilon = \overline{\Omega} \setminus \mathcal{S}_\epsilon.$$

- **Step 1, Estimate on $\mathcal{K}_\epsilon$:**

$$\sum_{x_i, x_j \in \mathcal{K}_\epsilon} k_{ij}(s_i - s_j)^2 \left| \frac{\boldsymbol{n}_i - \boldsymbol{n}_j}{2} \right|^2 \leq C \left(\max_{\substack{x_i, x_j \in \mathcal{K}_\epsilon, \\ |x_i - x_j| \leq h}} |\boldsymbol{n}_i - \boldsymbol{n}_j|^2 \right) \int_\Omega |\nabla s_h|^2 dx.$$

- **Step 2, Estimate on $\mathcal{S}_\epsilon$:**

$$\sum_{\text{either } x_i \text{ or } x_j \in \mathcal{S}_\epsilon} k_{ij}(s_i - s_j)^2 \left| \frac{\boldsymbol{n}_i - \boldsymbol{n}_j}{2} \right|^2 \leq 2 \int_{\cup \omega_i} |\nabla s_h|^2 dx \leq 2 \int_{\mathcal{S}_{2\epsilon}} |\nabla s_h|^2 dx,$$

where $\cup \omega_i$ is taken over all nodes x_i in $\mathcal{S}_\epsilon$.

- Combining both estimates, we have

$$\mathcal{E} \leq \underbrace{C \left(\max_{\substack{x_i, x_j \in \mathcal{K}_\epsilon, \\ |x_i - x_j| \leq h}} |\boldsymbol{n}_i - \boldsymbol{n}_j|^2 \right)}_{O(h^2)} \int_{\mathcal{K}_\epsilon} |\nabla s_h|^2 dx + 2 \underbrace{\int_{\mathcal{S}_{2\epsilon}} |\nabla s_h|^2 dx}_{\to 0 \text{ as } \epsilon \to 0}.$$

Consistency of the Discrete Energy

Proof:

We divide Ω into two regions:

$$\mathcal{S}_\epsilon = \{x \in \Omega,\ |s(x)| < \epsilon\} \quad \text{and} \quad \mathcal{K}_\epsilon = \overline{\Omega} \setminus \mathcal{S}_\epsilon.$$

- **Step 1, Estimate on $\mathcal{K}_\epsilon$:**

$$\sum_{x_i, x_j \in \mathcal{K}_\epsilon} k_{ij}(s_i - s_j)^2 \left| \frac{\boldsymbol{n}_i - \boldsymbol{n}_j}{2} \right|^2 \leq C \left(\max_{\substack{x_i, x_j \in \mathcal{K}_\epsilon, \\ |x_i - x_j| \leq h}} |\boldsymbol{n}_i - \boldsymbol{n}_j|^2 \right) \int_\Omega |\nabla s_h|^2 dx.$$

- **Step 2, Estimate on $\mathcal{S}_\epsilon$:**

$$\sum_{\text{either } x_i \text{ or } x_j \in \mathcal{S}_\epsilon} k_{ij}(s_i - s_j)^2 \left| \frac{\boldsymbol{n}_i - \boldsymbol{n}_j}{2} \right|^2 \leq 2 \int_{\cup \omega_i} |\nabla s_h|^2 dx \leq 2 \int_{\mathcal{S}_{2\epsilon}} |\nabla s_h|^2 dx,$$

  where $\cup \omega_i$ is taken over all nodes x_i in $\mathcal{S}_\epsilon$.
- Combining both estimates, we have

$$\mathcal{E} \leq \underbrace{C \left(\max_{\substack{x_i, x_j \in \mathcal{K}_\epsilon, \\ |x_i - x_j| \leq h}} |\boldsymbol{n}_i - \boldsymbol{n}_j|^2 \right)}_{O(h^2)} \int_{\mathcal{K}_\epsilon} |\nabla s_h|^2 dx + 2 \underbrace{\int_{\mathcal{S}_{2\epsilon}} |\nabla s_h|^2 dx}_{\to 0 \text{ as } \epsilon \to 0}.$$

Limit-Inf Inequality

The **main issue** is dealing with the case $0 < \kappa < 1$.

Recall a previous result:

$$E_1^h[\Omega, s_h, \boldsymbol{n}_h] \geq (\kappa - 1) \int_\Omega |\nabla I_h|s_h||^2 dx + \int_\Omega |\nabla \tilde{\boldsymbol{u}}_h|^2 dx,$$

where $\tilde{\boldsymbol{u}}_h$ in U_h and $\tilde{\boldsymbol{u}}_h(x_i) = |s_h(x_i)|\boldsymbol{n}_h(x_i)$ for all nodes x_i.

- **Coercivity:** for all $\kappa > 0$, we have

$$E_1^h[\Omega, s_h, \boldsymbol{n}_h] \geq \min\{\kappa, 1\} \int_\Omega |\nabla \tilde{\boldsymbol{u}}_h|^2 dx \geq \min\{\kappa, 1\} \int_\Omega |\nabla I_h|s_h||^2 dx.$$

- **Weak Lower Semi-continuity:** Let $\boldsymbol{w}_h \in U_h$. The energy

$$\int_\Omega L_h(\boldsymbol{w}_h, \nabla \boldsymbol{w}_h) dx, \quad \text{where}$$

$$L_h(\boldsymbol{w}_h, \nabla \boldsymbol{w}_h) := (\kappa - 1)|\nabla I_h|\boldsymbol{w}_h||^2 + |\nabla \boldsymbol{w}_h|^2,$$

is weakly lower semi-continuous, i.e. we have

$$\liminf_{h \to 0} \int_\Omega L_h(\boldsymbol{w}_h, \nabla \boldsymbol{w}_h) dx \geq \int_\Omega (\kappa - 1)|\nabla|\boldsymbol{w}||^2 + |\nabla \boldsymbol{w}|^2 dx.$$

for any weakly convergent sequence $\boldsymbol{w}_h \rightharpoonup \boldsymbol{w}$ in the H^1 norm.

Limit-Inf Inequality

The **main issue** is dealing with the case $0 < \kappa < 1$.

Recall a previous result:

$$E_1^h[\Omega, s_h, \boldsymbol{n}_h] \geq (\kappa - 1) \int_\Omega |\nabla I_h|s_h||^2 dx + \int_\Omega |\nabla \tilde{\boldsymbol{u}}_h|^2 dx,$$

where $\tilde{\boldsymbol{u}}_h$ in U_h and $\tilde{\boldsymbol{u}}_h(x_i) = |s_h(x_i)|\boldsymbol{n}_h(x_i)$ for all nodes x_i.

- **Coercivity:** for all $\kappa > 0$, we have

$$E_1^h[\Omega, s_h, \boldsymbol{n}_h] \geq \min\{\kappa, 1\} \int_\Omega |\nabla \tilde{\boldsymbol{u}}_h|^2 dx \geq \min\{\kappa, 1\} \int_\Omega |\nabla I_h|s_h||^2 dx.$$

- **Weak Lower Semi-continuity:** Let $\boldsymbol{w}_h \in U_h$. The energy

$$\int_\Omega L_h(\boldsymbol{w}_h, \nabla \boldsymbol{w}_h) dx, \quad \text{where}$$

$$L_h(\boldsymbol{w}_h, \nabla \boldsymbol{w}_h) := (\kappa - 1)|\nabla I_h|\boldsymbol{w}_h||^2 + |\nabla \boldsymbol{w}_h|^2,$$

is weakly lower semi-continuous, i.e. we have

$$\liminf_{h \to 0} \int_\Omega L_h(\boldsymbol{w}_h, \nabla \boldsymbol{w}_h) dx \geq \int_\Omega (\kappa - 1)|\nabla|\boldsymbol{w}||^2 + |\nabla \boldsymbol{w}|^2 dx.$$

for any weakly convergent sequence $\boldsymbol{w}_h \rightharpoonup \boldsymbol{w}$ in the H^1 norm.

Numerical Experiment: (plane defect in $3d$)

Visualization of defect formation:

MOVIE

Weak Lower Semi-continuity

Proof:

Main Goal:
Show that

$$L_h(\boldsymbol{w}_h, \nabla \boldsymbol{w}_h) := (\kappa - 1)|\nabla I_h|\boldsymbol{w}_h||^2 + |\nabla \boldsymbol{w}_h|^2$$

is *convex with respect to* $\nabla \boldsymbol{w}_h$, even for $0 < \kappa < 1$.

Rewrite energy density:

- Suppose dimension is $d = 2$. Let T be a triangle in $\mathcal{T}_h$ with vertices x_0, x_1, x_2. Define

$$\boldsymbol{e}_i := x_i - x_0, \quad \text{for } i = 1, 2, \quad \boldsymbol{w}_i := \boldsymbol{w}_h(x_i) \quad \text{for } i = 0, 1, 2.$$

- A simple calculation gives:

$$\nabla \boldsymbol{w}_h = (\boldsymbol{w}_1 - \boldsymbol{w}_0) \otimes \boldsymbol{e}_1^* + (\boldsymbol{w}_2 - \boldsymbol{w}_0) \otimes \boldsymbol{e}_2^*,$$
$$\nabla I_h|\boldsymbol{w}_h| = (|\boldsymbol{w}_1| - |\boldsymbol{w}_0|)\boldsymbol{e}_1^* + (|\boldsymbol{w}_2| - |\boldsymbol{w}_0|)\boldsymbol{e}_2^*,$$

  where $\boldsymbol{e}_i \cdot \boldsymbol{e}_j^* = \delta_{ij}$ (dual basis).

- Note:

$$|\boldsymbol{w}_i| - |\boldsymbol{w}_0| = \frac{\boldsymbol{w}_i + \boldsymbol{w}_0}{|\boldsymbol{w}_i| + |\boldsymbol{w}_0|} \cdot (\boldsymbol{w}_i - \boldsymbol{w}_0).$$

Weak Lower Semi-continuity

Proof:

Main Goal:
Show that

$$L_h(\boldsymbol{w}_h, \nabla \boldsymbol{w}_h) := (\kappa - 1)|\nabla I_h|\boldsymbol{w}_h||^2 + |\nabla \boldsymbol{w}_h|^2$$

is *convex with respect to* $\nabla \boldsymbol{w}_h$, even for $0 < \kappa < 1$.

Rewrite energy density:

- Suppose dimension is $d = 2$. Let T be a triangle in $\mathcal{T}_h$ with vertices x_0, x_1, x_2. Define

$$\boldsymbol{e}_i := x_i - x_0, \quad \text{for } i = 1, 2, \quad \boldsymbol{w}_i := \boldsymbol{w}_h(x_i) \quad \text{for } i = 0, 1, 2.$$

- A simple calculation gives:

$$\nabla \boldsymbol{w}_h = (\boldsymbol{w}_1 - \boldsymbol{w}_0) \otimes \boldsymbol{e}_1^* + (\boldsymbol{w}_2 - \boldsymbol{w}_0) \otimes \boldsymbol{e}_2^*,$$
$$\nabla I_h|\boldsymbol{w}_h| = (|\boldsymbol{w}_1| - |\boldsymbol{w}_0|)\boldsymbol{e}_1^* + (|\boldsymbol{w}_2| - |\boldsymbol{w}_0|)\boldsymbol{e}_2^*,$$

  where $\boldsymbol{e}_i \cdot \boldsymbol{e}_j^* = \delta_{ij}$ (dual basis).
- Note:

$$|\boldsymbol{w}_i| - |\boldsymbol{w}_0| = \frac{\boldsymbol{w}_i + \boldsymbol{w}_0}{|\boldsymbol{w}_i| + |\boldsymbol{w}_0|} \cdot (\boldsymbol{w}_i - \boldsymbol{w}_0).$$

Weak Lower Semi-continuity

Proof:

- Therefore,
$$\nabla I_h|\boldsymbol{w}_h| = G_h(\boldsymbol{w}_h) : \nabla \boldsymbol{w}_h,$$
where G_h is a 3-tensor:
$$G_h(\boldsymbol{w}_h) := \frac{\boldsymbol{w}_1 + \boldsymbol{w}_0}{|\boldsymbol{w}_1| + |\boldsymbol{w}_0|} \otimes \boldsymbol{e}_1 \otimes \boldsymbol{e}_1^* + \frac{\boldsymbol{w}_2 + \boldsymbol{w}_0}{|\boldsymbol{w}_2| + |\boldsymbol{w}_0|} \otimes \boldsymbol{e}_2 \otimes \boldsymbol{e}_2^*.$$
- We define $(\boldsymbol{g}_1 \otimes \boldsymbol{g}_2 \otimes \boldsymbol{g}_3) : (\boldsymbol{m}_1 \otimes \boldsymbol{m}_2) = (\boldsymbol{g}_1 \cdot \boldsymbol{m}_1)(\boldsymbol{g}_2 \cdot \boldsymbol{m}_2)\boldsymbol{g}_3$.
- Hence,
$$L_h(\boldsymbol{w}_h, \nabla \boldsymbol{w}_h) = |\nabla \boldsymbol{w}_h|^2 + (\kappa - 1)|G_h : \nabla \boldsymbol{w}_h|^2.$$

Note:

- $\boldsymbol{e}_1 \otimes \boldsymbol{e}_1^* + \boldsymbol{e}_2 \otimes \boldsymbol{e}_2^* = I$, i.e. the identity matrix.
- If $\boldsymbol{w}_h \to \boldsymbol{w}$ a.e., then, for a.e. x such that $\boldsymbol{w}(x) \neq \mathbf{0}$,
$$\frac{\boldsymbol{w}_i + \boldsymbol{w}_0}{|\boldsymbol{w}_i| + |\boldsymbol{w}_0|} \to \frac{\boldsymbol{w}}{|\boldsymbol{w}|}, \quad \text{for } i = 1,2 \quad \Rightarrow \quad G_h \to G(\boldsymbol{w}) := \frac{\boldsymbol{w}}{|\boldsymbol{w}|} \otimes I.$$

Weak Lower Semi-continuity

Proof:

- Therefore,
$$\nabla I_h|\boldsymbol{w}_h| = G_h(\boldsymbol{w}_h) : \nabla \boldsymbol{w}_h,$$
where G_h is a 3-tensor:
$$G_h(\boldsymbol{w}_h) := \frac{\boldsymbol{w}_1 + \boldsymbol{w}_0}{|\boldsymbol{w}_1| + |\boldsymbol{w}_0|} \otimes \boldsymbol{e}_1 \otimes \boldsymbol{e}_1^* + \frac{\boldsymbol{w}_2 + \boldsymbol{w}_0}{|\boldsymbol{w}_2| + |\boldsymbol{w}_0|} \otimes \boldsymbol{e}_2 \otimes \boldsymbol{e}_2^*.$$
- We define $(\boldsymbol{g}_1 \otimes \boldsymbol{g}_2 \otimes \boldsymbol{g}_3) : (\boldsymbol{m}_1 \otimes \boldsymbol{m}_2) = (\boldsymbol{g}_1 \cdot \boldsymbol{m}_1)(\boldsymbol{g}_2 \cdot \boldsymbol{m}_2)\boldsymbol{g}_3$.
- Hence,
$$L_h(\boldsymbol{w}_h, \nabla \boldsymbol{w}_h) = |\nabla \boldsymbol{w}_h|^2 + (\kappa - 1)|G_h : \nabla \boldsymbol{w}_h|^2.$$

Note:

- $\boldsymbol{e}_1 \otimes \boldsymbol{e}_1^* + \boldsymbol{e}_2 \otimes \boldsymbol{e}_2^* = I$, i.e. the identity matrix.
- If $\boldsymbol{w}_h \to \boldsymbol{w}$ a.e., then, for a.e. x such that $\boldsymbol{w}(x) \neq \boldsymbol{0}$,
$$\frac{\boldsymbol{w}_i + \boldsymbol{w}_0}{|\boldsymbol{w}_i| + |\boldsymbol{w}_0|} \to \frac{\boldsymbol{w}}{|\boldsymbol{w}|}, \quad \text{for } i = 1, 2 \quad \Rightarrow \quad G_h \to G(\boldsymbol{w}) := \frac{\boldsymbol{w}}{|\boldsymbol{w}|} \otimes I.$$

Weak Lower Semi-continuity

Proof:

- **Claim:** the energy density

$$L(\boldsymbol{w}, M) := |M|^2 + (\kappa - 1)|G(\boldsymbol{w}) : M|^2$$

  is convex with respect to any matrix M.
- Indeed, $L(\boldsymbol{w}, M)$ is quadratic in M, so we only need to show that $L(\boldsymbol{w}, M) > 0$ for any M.
- This is equivalent to showing $|G : M| \leq |M|$, which follows by simple inequalities.
- A similar argument shows that $L_h(\boldsymbol{w}_h, M) > 0$ for any matrix M, and so also convex.

For the remainder of the proof, letting $\boldsymbol{w}_h$ be a weakly convergent sequence in $H^1(\Omega)$, and applying standard limiting arguments, we get the assertion.

Weak Lower Semi-continuity

Proof:

- **Claim:** the energy density
$$L(\boldsymbol{w}, M) := |M|^2 + (\kappa - 1)|G(\boldsymbol{w}) : M|^2$$
is convex with respect to any matrix M.
- Indeed, $L(\boldsymbol{w}, M)$ is quadratic in M, so we only need to show that $L(\boldsymbol{w}, M) > 0$ for any M.
- This is equivalent to showing $|G : M| \leq |M|$, which follows by simple inequalities.
- A similar argument shows that $L_h(\boldsymbol{w}_h, M) > 0$ for any matrix M, and so also convex.

For the remainder of the proof, letting $\boldsymbol{w}_h$ be a weakly convergent sequence in $H^1(\Omega)$, and applying standard limiting arguments, we get the assertion.

Weak Lower Semi-continuity

Proof:

- **Claim:** the energy density

$$L(\boldsymbol{w}, M) := |M|^2 + (\kappa - 1)|G(\boldsymbol{w}) : M|^2$$

  is convex with respect to any matrix M.
- Indeed, $L(\boldsymbol{w}, M)$ is quadratic in M, so we only need to show that $L(\boldsymbol{w}, M) > 0$ for any M.
- This is equivalent to showing $|G : M| \leq |M|$, which follows by simple inequalities.
- A similar argument shows that $L_h(\boldsymbol{w}_h, M) > 0$ for any matrix M, and so also convex.

For the remainder of the proof, letting $\boldsymbol{w}_h$ be a weakly convergent sequence in $H^1(\Omega)$, and applying standard limiting arguments, we get the assertion.

Limit-Inf Inequality

Proof:

- Let $\{(s_h, \boldsymbol{n}_h)\}$ be any sequence converging strongly to $(s, \boldsymbol{n})$ in L^2.
- We know that the H^1 norms of $I_h|s_h|$ and $\tilde{\boldsymbol{u}}_h$ are bounded.
- Extract a subsequence $\{(I_h|s_h|, \tilde{\boldsymbol{u}}_h)\}$ converging weakly in H^1 and strongly in L^2 to $(|s|, \tilde{\boldsymbol{u}})$.
- Moreover, one can show $\tilde{\boldsymbol{u}}(x) = |s(x)|\boldsymbol{n}(x)$, with $|\boldsymbol{n}(x)| = 1$, for a.e. x.

By previous results and weak lower semi-continuity:

$$\begin{aligned}
\liminf_{h\to 0} E_1^h[s_h, \boldsymbol{n}_h] &\geq \int_\Omega (\kappa - 1)|\nabla|\tilde{\boldsymbol{u}}||^2 + |\nabla \tilde{\boldsymbol{u}}|^2 dx \\
&= \int_\Omega \kappa |\nabla |s||^2 + |s|^2 |\nabla \boldsymbol{n}|^2 dx \\
&= \int_\Omega \kappa |\nabla s|^2 + s^2 |\nabla \boldsymbol{n}|^2 dx \\
&= E_1[s, \boldsymbol{n}].
\end{aligned}$$

Limit-Inf Inequality

Proof:

- Let $\{(s_h, \boldsymbol{n}_h)\}$ be any sequence converging strongly to $(s, \boldsymbol{n})$ in L^2.
- We know that the H^1 norms of $I_h|s_h|$ and $\tilde{\boldsymbol{u}}_h$ are bounded.
- Extract a subsequence $\{(I_h|s_h|, \tilde{\boldsymbol{u}}_h)\}$ converging weakly in H^1 and strongly in L^2 to $(|s|, \tilde{\boldsymbol{u}})$.
- Moreover, one can show $\tilde{\boldsymbol{u}}(x) = |s(x)|\boldsymbol{n}(x)$, with $|\boldsymbol{n}(x)| = 1$, for a.e. x.

By previous results and weak lower semi-continuity:

$$\begin{aligned}
\liminf_{h \to 0} E_1^h[s_h, \boldsymbol{n}_h] &\geq \int_\Omega (\kappa - 1)|\nabla|\tilde{\boldsymbol{u}}||^2 + |\nabla \tilde{\boldsymbol{u}}|^2 dx \\
&= \int_\Omega \kappa|\nabla|s||^2 + |s|^2|\nabla \boldsymbol{n}|^2 dx \\
&= \int_\Omega \kappa|\nabla s|^2 + s^2|\nabla \boldsymbol{n}|^2 dx \\
&= E_1[s, \boldsymbol{n}].
\end{aligned}$$

OUTLINE

Alternating Direction Method

- We design a gradient flow to seek a minimizer $(S, \boldsymbol{N})$ of the discrete energy $E^h[S, \boldsymbol{N}]$.
- Given the k-th iteration $(S^k, \boldsymbol{N}^k)$, to respect the unit length constraint for $\boldsymbol{N}^{k+1}$ at all nodes, we consider a first order variation with respect to $\boldsymbol{N}^k$ in the **discrete tangent space** [Alouges 97, Bartels 10]:

$$\mathbb{T}_h^k = \{\boldsymbol{T} \in H^1(\Omega), \boldsymbol{T}|_T \text{ is affine, and } \boldsymbol{T}_i \cdot \boldsymbol{N}_i^k = 0 \text{ for all nodes } x_i\}.$$

- **Step (a):** find $\boldsymbol{T}^k$ in $\mathbb{T}_h^k$ such that for any $\boldsymbol{V}$ in $\mathbb{T}_h^k$ we have

$$\delta_{\boldsymbol{N}} E_1^h[S^k, \boldsymbol{N}^k + \boldsymbol{T}^k; \boldsymbol{V}] = 0.$$

- **Step (b):** normalize:

$$\boldsymbol{N}_i^{k+1} := \frac{\boldsymbol{N}_i^k + \boldsymbol{T}_i^k}{|\boldsymbol{N}_i^k + \boldsymbol{T}_i^k|}, \quad \text{at all nodes.}$$

- **Step (c):** find S^{k+1} in W_h such that for any $Z_h \in W_h$ we have

$$\int_\Omega \frac{S_h^{k+1} - S_h^k}{\delta t} Z_h = -\delta_S E_1^h[S_h^{k+1}, \boldsymbol{N}_h^{k+1}; Z_h] - \delta_S E_2^h[S_h^{k+1}; Z_h].$$

Alternating Direction Method

- We design a gradient flow to seek a minimizer $(S, \boldsymbol{N})$ of the discrete energy $E^h[S, \boldsymbol{N}]$.
- Given the k-th iteration $(S^k, \boldsymbol{N}^k)$, to respect the unit length constraint for $\boldsymbol{N}^{k+1}$ at all nodes, we consider a first order variation with respect to $\boldsymbol{N}^k$ in the **discrete tangent space** [Alouges 97, Bartels 10]:

$$\mathbb{T}_h^k = \{\boldsymbol{T} \in H^1(\Omega), \boldsymbol{T}|_T \text{ is affine, and } \boldsymbol{T}_i \cdot \boldsymbol{N}_i^k = 0 \text{ for all nodes } x_i\}.$$

- **Step (a):** find $\boldsymbol{T}^k$ in $\mathbb{T}_h^k$ such that for any $\boldsymbol{V}$ in $\mathbb{T}_h^k$ we have

$$\delta_{\boldsymbol{N}} E_1^h[S^k, \boldsymbol{N}^k + \boldsymbol{T}^k; \boldsymbol{V}] = 0.$$

- **Step (b):** normalize:

$$\boldsymbol{N}_i^{k+1} := \frac{\boldsymbol{N}_i^k + \boldsymbol{T}_i^k}{|\boldsymbol{N}_i^k + \boldsymbol{T}_i^k|}, \quad \text{at all nodes.}$$

- **Step (c):** find S^{k+1} in W_h such that for any $Z_h \in W_h$ we have

$$\int_\Omega \frac{S_h^{k+1} - S_h^k}{\delta t} Z_h = -\delta_S E_1^h[S_h^{k+1}, \boldsymbol{N}_h^{k+1}; Z_h] - \delta_S E_2^h[S_h^{k+1}; Z_h].$$

Alternating Direction Method

- We design a gradient flow to seek a minimizer $(S, \boldsymbol{N})$ of the discrete energy $E^h[S, \boldsymbol{N}]$.
- Given the k-th iteration $(S^k, \boldsymbol{N}^k)$, to respect the unit length constraint for $\boldsymbol{N}^{k+1}$ at all nodes, we consider a first order variation with respect to $\boldsymbol{N}^k$ in the **discrete tangent space** [Alouges 97, Bartels 10]:

$$\mathbb{T}_h^k = \{\boldsymbol{T} \in H^1(\Omega), \boldsymbol{T}|_T \text{ is affine, and } \boldsymbol{T}_i \cdot \boldsymbol{N}_i^k = 0 \text{ for all nodes } x_i\}.$$

- **Step (a):** find $\boldsymbol{T}^k$ in $\mathbb{T}_h^k$ such that for any $\boldsymbol{V}$ in $\mathbb{T}_h^k$ we have

$$\delta_{\boldsymbol{N}} E_1^h[S^k, \boldsymbol{N}^k + \boldsymbol{T}^k; \boldsymbol{V}] = 0.$$

- **Step (b):** normalize:

$$\boldsymbol{N}_i^{k+1} := \frac{\boldsymbol{N}_i^k + \boldsymbol{T}_i^k}{|\boldsymbol{N}_i^k + \boldsymbol{T}_i^k|}, \qquad \text{at all nodes.}$$

- **Step (c):** find S^{k+1} in W_h such that for any $Z_h \in W_h$ we have

$$\int_\Omega \frac{S_h^{k+1} - S_h^k}{\delta t} Z_h = -\delta_S E_1^h[S_h^{k+1}, \boldsymbol{N}_h^{k+1}; Z_h] - \delta_S E_2^h[S_h^{k+1}; Z_h].$$

Alternating Direction Method

- We design a gradient flow to seek a minimizer $(S, \boldsymbol{N})$ of the discrete energy $E^h[S, \boldsymbol{N}]$.
- Given the k-th iteration $(S^k, \boldsymbol{N}^k)$, to respect the unit length constraint for $\boldsymbol{N}^{k+1}$ at all nodes, we consider a first order variation with respect to $\boldsymbol{N}^k$ in the **discrete tangent space** [Alouges 97, Bartels 10]:

$$\mathbb{T}_h^k = \{\boldsymbol{T} \in H^1(\Omega), \boldsymbol{T}|_T \text{ is affine, and } \boldsymbol{T}_i \cdot \boldsymbol{N}_i^k = 0 \text{ for all nodes } x_i\}.$$

- **Step (a):** find $\boldsymbol{T}^k$ in $\mathbb{T}_h^k$ such that for any $\boldsymbol{V}$ in $\mathbb{T}_h^k$ we have

$$\delta_{\boldsymbol{N}} E_1^h[S^k, \boldsymbol{N}^k + \boldsymbol{T}^k; \boldsymbol{V}] = 0.$$

- **Step (b):** normalize:

$$\boldsymbol{N}_i^{k+1} := \frac{\boldsymbol{N}_i^k + \boldsymbol{T}_i^k}{|\boldsymbol{N}_i^k + \boldsymbol{T}_i^k|}, \qquad \text{at all nodes.}$$

- **Step (c):** find S^{k+1} in W_h such that for any $Z_h \in W_h$ we have

$$\int_\Omega \frac{S_h^{k+1} - S_h^k}{\delta t} Z_h = -\delta_S E_1^h[S_h^{k+1}, \boldsymbol{N}_h^{k+1}; Z_h] - \delta_S E_2^h[S_h^{k+1}; Z_h].$$

Alternating Direction Method

- We design a gradient flow to seek a minimizer $(S, \boldsymbol{N})$ of the discrete energy $E^h[S, \boldsymbol{N}]$.
- Given the k-th iteration $(S^k, \boldsymbol{N}^k)$, to respect the unit length constraint for $\boldsymbol{N}^{k+1}$ at all nodes, we consider a first order variation with respect to $\boldsymbol{N}^k$ in the **discrete tangent space** [Alouges 97, Bartels 10]:

$$\mathbb{T}_h^k = \{\boldsymbol{T} \in H^1(\Omega), \boldsymbol{T}|_T \text{ is affine, and } \boldsymbol{T}_i \cdot \boldsymbol{N}_i^k = 0 \text{ for all nodes } x_i\}.$$

- **Step (a):** find $\boldsymbol{T}^k$ in $\mathbb{T}_h^k$ such that for any $\boldsymbol{V}$ in $\mathbb{T}_h^k$ we have

$$\delta_{\boldsymbol{N}} E_1^h[S^k, \boldsymbol{N}^k + \boldsymbol{T}^k; \boldsymbol{V}] = 0.$$

- **Step (b):** normalize:

$$\boldsymbol{N}_i^{k+1} := \frac{\boldsymbol{N}_i^k + \boldsymbol{T}_i^k}{|\boldsymbol{N}_i^k + \boldsymbol{T}_i^k|}, \qquad \text{at all nodes.}$$

- **Step (c):** find S^{k+1} in W_h such that for any $Z_h \in W_h$ we have

$$\int_\Omega \frac{S_h^{k+1} - S_h^k}{\delta t} Z_h = -\delta_S E_1^h[S_h^{k+1}, \boldsymbol{N}_h^{k+1}; Z_h] - \delta_S E_2^h[S_h^{k+1}; Z_h].$$

Monotone Energy Decrease

- **Energy decrease of the gradient flow:**
  Given a pair $(\boldsymbol{N}_h^k, S_h^k)$, let $(\boldsymbol{N}_h^{k+1}, S_h^{k+1})$ be the discrete gradient flow obtained by the algorithm above. Then

$$E^h[S_h^{k+1}, \boldsymbol{N}_h^{k+1}] \le E^h[S_h^k, \boldsymbol{N}_h^k].$$

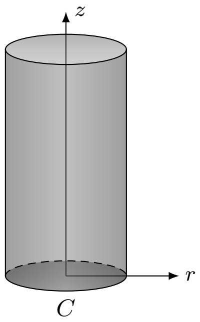
  Equality holds if and only if the flow $(\boldsymbol{N}_h^k, S_h^k)$ attains an equilibrium state, that is,

$$(\boldsymbol{N}_h^{k+1}, S_h^{k+1}) = (\boldsymbol{N}_h^k, S_h^k).$$

- Proof is essentially based on linear arguments, except for step (b) which uses an argument from [Alouges 97, Bartels 10].

OUTLINE

Fluting effect and line defect



- We neglect the double well potential ψ_B.
- Consider the minimizers of

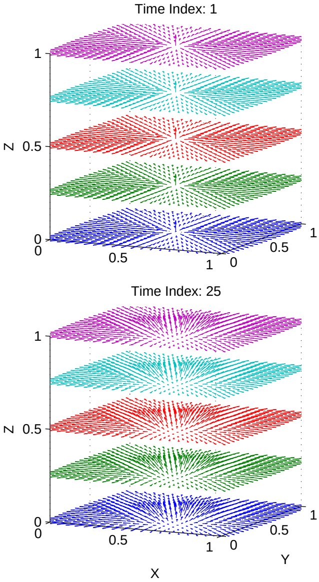
$$E = \int_C \kappa|\nabla s|^2 + s^2|\nabla \boldsymbol{n}|^2 dx.$$

- Boundary condition:

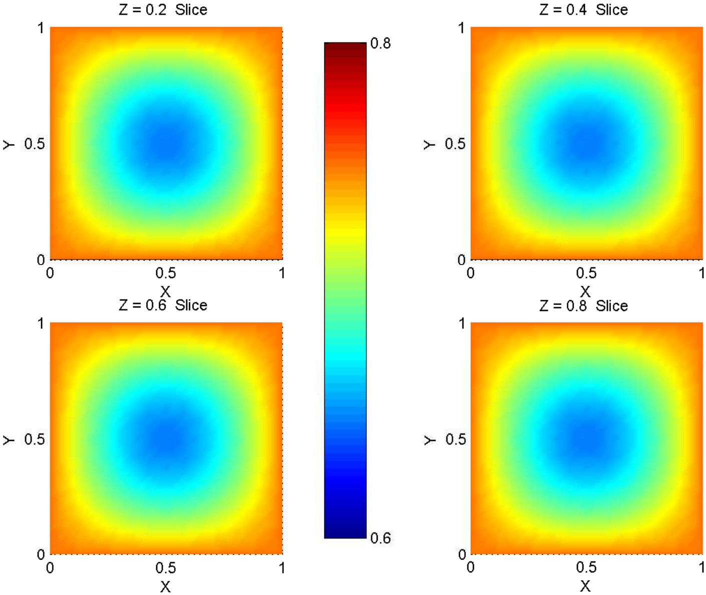
$$s|_{\mathcal{S}_0} = s_0 > 0 \quad \text{and } \boldsymbol{n}|_{\mathcal{S}_0} = \frac{\boldsymbol{r}}{|\boldsymbol{r}|}.$$

- Theorem [Characterization of singular set, Mizel Roccato Virga1991]: If $(s, \boldsymbol{n})$ is the minimizer of energy E, then either the singular set $\mathcal{S}$ is empty or $\mathcal{S} = \{|\boldsymbol{r}| = 0\}$.

Numerical Experiments: $\kappa = 10$ Fluting effect

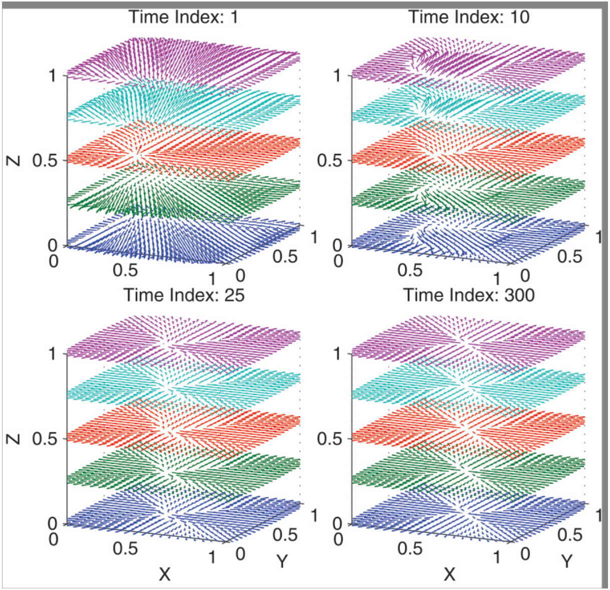


Numerical Experiments: $\kappa = 10$ Fluting effect



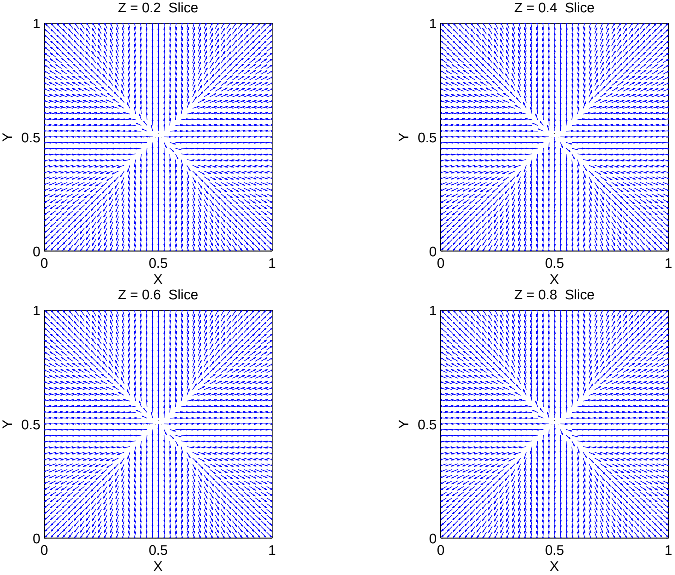
Numerical Experiments: $\kappa = 0.1$ "Propeller" Defect

MOVIE



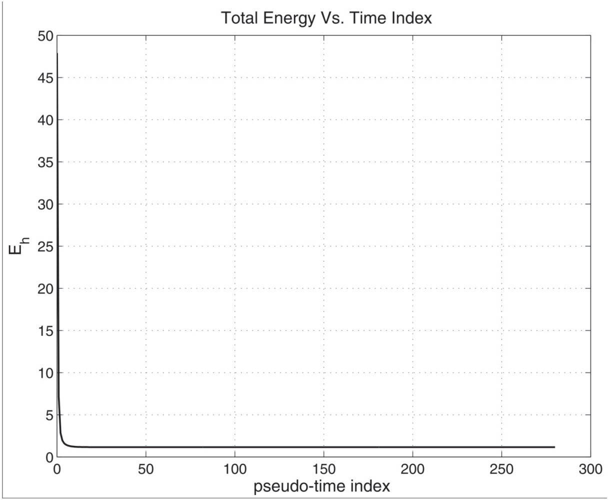
Numerical Experiments: $\kappa = 0.1$ "Propeller" Defect

MOVIE



Numerical Experiments: $\kappa = 0.1$ "Propeller" Defect

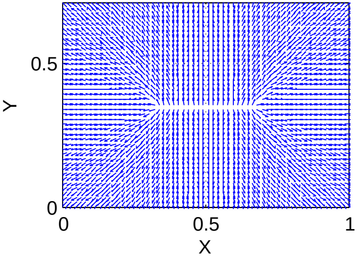
Energy Decrease:

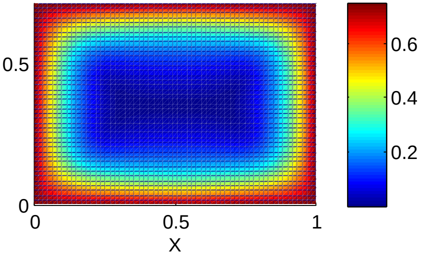


Numerical Experiments: $\kappa = 0.1$ Defect In A Rectangular Box

MOVIE: Director Field

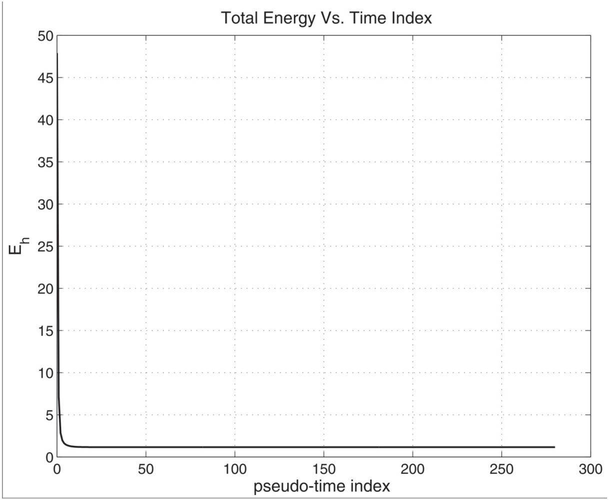
MOVIE: Defect Evolution





Numerical Experiments: $\kappa = 0.1$ Defect In A Rectangular Box

Energy Decrease:



Conclusion

- We have a finite element method (FEM) for the one constant Ericksen's model:
$$E := \int_\Omega \kappa|\nabla s|^2 + s^2|\nabla \boldsymbol{n}|^2 dx + \int_\Omega \psi_B(s) dx.$$
- We have Γ-convergence of the FEM.
- We have monotone energy decrease of the gradient flow.
- Our FEM is capable of capturing high dimensional defects.

Future Work:

- Include magnetic (electric) field to manipulate the liquid crystal.
- Investigate the Q-tensor method.
- Study flows of liquid crystals (couple Ericksen's model with Stokes flow).