TECHNISCHE UNIVERSITÄT DRESDEN

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DFG Research Unit 3013 - Vector- and Tensor-Valued Surface PDEs

Bending plates of nematic liquid crystal elastomers

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1. Problem statement

Programmable actuators provide a wide range of modern applications, particularly at small scales. We focus on a class of thin bilayers which are made out of nematic liquid crystal elastomers. Concepts from hyperelasticity and Landau-de Gennes theory lead to an energy functional for a deformation y and a director field n:

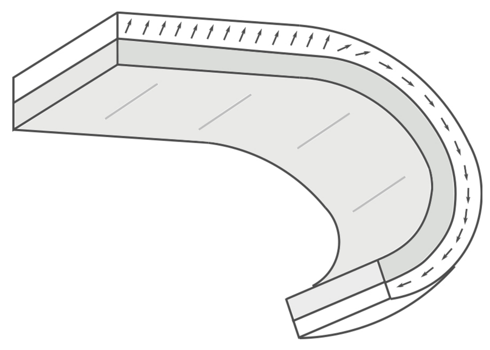
$$\mathcal{E}_h(y,n) := \frac{1}{h^3}\int_{\Omega_h} W(A(n)^{-\frac{1}{2}}(\nabla y)A(n_0)^{-\frac{1}{2}}) + \frac{\varepsilon}{h^3}\int_{\Omega_h} |\nabla n(\nabla y)^{-1}|^2 \det \nabla y.$$

The functional involves the following quantities:

- stored energy density : W
- thin reference domain : $\Omega_h = S \times (-\frac{h}{2}, \frac{h}{2})$
- step length tensor :

$$A(n) = \begin{cases} I_{3\times 3} + r(-\frac{1}{3}I_{3\times 3} + n\otimes n) & \text{, where } x_3 > 0 \\ I_{3\times 3} & \text{, where } x_3 < 0 \end{cases}$$

- scaling: $0 < h \ll 1$, $\varepsilon \sim h^2\bar{\varepsilon}$, $r \sim h\bar{r}$



For an efficient numerical simulation it is desirable to derive a dimensionally reduced model reflecting the limit $h \to 0$ of very thin plates for bounded energies. The variational limit is an extended nonlinear bending theory that specifies the deformation of the midplane and the director field:

$$\mathcal{E}(y,n) := \frac{1}{24}\int_S Q_2(II + Z(\nabla' y^T n)) + \frac{1}{64}\int_S Q_2(Z(\nabla' y^T n)) + \frac{\bar{\varepsilon}}{2}\int_S |\nabla' n|^2.$$

The reduced functional involves the following quantities:

- Q is a quadratic form obtained from the second variation of W at identity .
- II is the second fundamental form of the isometrically deformed surface $y(S)$.
- $Z(\nabla' y^T n)$ is a spontaneous curvature tensor determined by n.

The derivation is carried out by Gamma-convergece. (See points 2 and 3.)

2. Compactness and Liminf-Inequality

- Compactness of Deformations: Bounded energy $\limsup_{h\searrow 0}\mathcal{E}_h(y_h,n_h) < \infty$ implies (see [Schmidt '07]):

$$\exists y \in W^{2,2}_{iso}(S,\mathbb{R}^3): \quad \nabla y_h \xrightarrow{L^2} (\partial_1 y, \partial_2 y, \partial_1 y \times \partial_2 y).$$

- Compactness of Directors: Assume for some $q > 4$,

$$W(F) \geq \frac{1}{c}|F|^q - c$$

$$W(F) \geq \begin{cases} \frac{1}{c}\frac{1}{\sqrt{\det(F)}^q} - c, & \det F > 0 \\ \infty, & \det F \leq 0. \end{cases}$$

Then, $\limsup_{h\searrow 0}\mathcal{E}_h(y_h,n_h) < \infty$ implies (for some $p \in (1,2)$)

$$\exists n \in W^{1,2}(S,\mathbb{S}^2): \quad n_h \xrightarrow{W^{1,p}} n.$$

- Liminf-inequality: For y, n as above: $\liminf_{h\searrow}\mathcal{E}_h(y_h,n_h) \geq \mathcal{E}(y,n)$. See [Schmidt '07]. (The additional director field in the model poses no big problems.)

3. Recovery Sequence

First, we approximate any $W^{2,2}$-isometric immersion of S by suitable $y \in C^\infty_{\mathrm{iso}}(S,\mathbb{R}^3)$. For these y, the ansatz is (see [Schmidt '07] and [Padilla-Garza '20])

$$y_h(x',x_3) = (1-hC)\,[y(x') + x_3 b(x')] + \sqrt{h}R(x')\begin{pmatrix} -x_3\partial_1 v(x') \\ -x_3\partial_2 v(x') \\ v(x') \end{pmatrix} + hg(x') + O(h^2)!$$

$$n(x',x_3) = n(x')$$

Here:

- $b = \partial_1 y \times \partial_2 y$ and $R = (\partial_1 y, \partial_2 y, b)$.
- $C > 0$ is constant.
- $\operatorname{supp} v \subseteq \{II = 0\}$.

The red terms are introduced as a wrinkling ansatz with compression. Note the high order ($\sqrt{h}$) of out-of-plane wrinkling. Also note that the compression affects $\{II \neq 0\}$ as well, in order to obtain a smooth ansatz.

4. Boundary Conditions and open Questions

We want to consider clamped 3D-boundary conditions of the form

$$(BC_3) \qquad y_h(x',x_3) = (1-hC)\begin{pmatrix} x' \\ x_3 \end{pmatrix} \text{ for all } (x',x_3) \in \Gamma \times \left(-\frac{h}{2}, \frac{h}{2}\right)$$

for some $\Gamma \subseteq \partial S$. The fitting 2D-boundary condition is

$$(BC_2) \qquad \left.\begin{aligned} y(x') &= \begin{pmatrix} x' \\ 0 \end{pmatrix} \\ \nabla' y(x') &= \begin{pmatrix} I_{2\times 2} \\ 0\ 0 \end{pmatrix} \end{aligned}\right\} \text{ for all } x' \in \Gamma$$

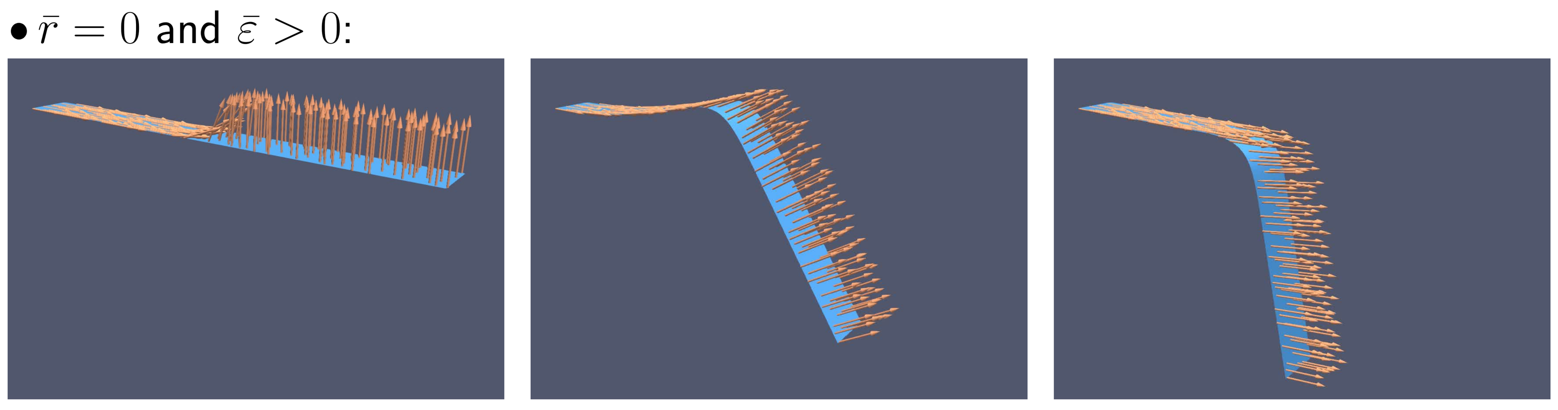
But then, in the recovery sequence's construction, questions arise:

- We need to adapt the results of [Pakzad '04] and [Hornung '11] such that every $y \in W^{2,2}_{\mathrm{iso}}(S,\mathbb{R}^3)$ satisfying (BC_2) is approximated by a smooth isometric immersion also satisfying (BC_2). This can be done as in [Neukamm, Olbermann '15].
- The compression $(1-hC)$, which is important for the wrinkling ansatz, is reflected in (BC_3). How to get rid of it? The solution might be a small transition layer connecting a non-compressed Dirichlet boundary with a compressed major part of the body.

5. Numerical Experiments

Simulation 1

- Done by Christian Palus and Sören Bartels.
- Deformation clamped at left edge.
- Director field fixed in Lagrangian coordinates.
- Minimization of the 2D-energy via gradient flow.
- $\bar{r} = 0$ and $\bar{\varepsilon} > 0$:



Simulation 2

- Deformation fixed at opposing edges.
- Director field is free.
- Assuming all quantities to be independent of x_2-direction.
- Applying body force.
- Drawing only representative middle line: