# Frank energy for nematic elastomers: a nonlinear model

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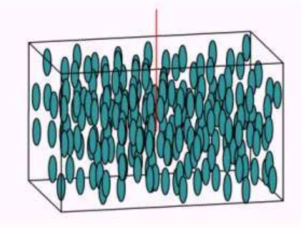
- **M. B. & A. DeSimone**. Frank energy for nematic elastomers: a nonlinear model. Preprint.

http://cvgmt.sns.it/people/barchiesi/

# Nematic elastomers

Nematic Elastomers are rubbery networks composed of long, crosslinked polymer chains. They have one axis that is longer and preferred, with the other two being equivalent (can be approximated as cylinders).
Their mechanical response is governed by the coupling of rubber elasticity with the orientational order of the molecules.



# Energy describing nematic elastomers

As implementation of the Warner-Terentjev model for nematic elastomers, DeSimone-Teresi have proposed the following variational nonlinear model:

$$\mathcal{I}(u,\mathbf{n}) := \int_{u(\Omega)} |\nabla \mathbf{n}(y)|^2 dy + \int_{\Omega} W_{\mathrm{mec}}\big(\nabla u(x), \mathbf{n}(u(x))\big)\, dx$$

- $u : \Omega \to \mathbb{R}^3$ is a deformations of a body whose reference configuration is $\Omega \subset \mathbb{R}^3$;
- $\mathbf{n} : u(\Omega) \to \mathbb{S}^2$ is the director field describing the nematic order in the elastomer.

The Frank energy penalizes spatial variations of the nematic director.

The point is that it has been typically evaluated in the reference configuration while, when large deformations are in order, it is more natural to consider spatial variations in the deformed configuration.

### Goal

*Today we will see (under reasonable assumptions) the existence of minimal energy states when the Frank term is written in the deformed configuration.*

# Coupling between deformation and nematic order

Here

$$W_{\mathrm{mec}}(F, \mathbf{n}) := \widetilde{W}(V_{\mathbf{n}}^{-1} F),$$

where $\widetilde{W} : \{F \in \mathbb{R}^{3\times 3} : \det F = 1\} \to [0, \infty)$ is a polyconvex energy and $V_{\mathbf{n}}$ is the stretch in the direction $\mathbf{n} \in \mathbb{S}^2$ of a fixed amplitude $\alpha > 0$.

# Difficulties

The difficulty here is that our energy functional has two terms, the Frank one defined on the deformed configuration, and the mechanical one defined on the reference configuration.

We need to push-forward the second one in order to work on the same domain. For this task, it is necessary that the inverse of the deformation has some regularity properties.

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Note also that

- in general $u(\Omega)$ is not open;
- the composition $\mathbf{n} \circ u$ is not measurable;
- $u_k \to u$ does not imply $\chi_{u_k(\Omega)} \to \chi_{u(\Omega)}$;
- $u_k \to u$ and $\mathbf{n}_k \to \mathbf{n}$ do not imply $\mathbf{n}_k \circ u_k \to \mathbf{n} \circ u$.

# Ambient space of our problem

The deformations belong to

$$\mathcal{W}(\Omega, \mathbb{R}^3) := \left\{ u \in W^{1,3}(\Omega, \mathbb{R}^3) : \ \det \nabla u = 1 \text{ a.e. in } \Omega \right\}.$$

**Remark**

*A function $u \in \mathcal{W}(\Omega, \mathbb{R}^3)$ has nice properties: firstly, it is continuous and differentiable a.e. in $\Omega$. Moreover, it satisfies the N property ($|u(D)| = 0$ whenever $D \subset \Omega$ is a measurable set such that $|D| = 0$), and the $N^{-1}$ property ($|u^{-1}(D)| = 0$ whenever $D \subset \mathbb{R}^3$ is a measurable set such that $|D| = 0$).*

**Remark**

*More important, $u$ is almost locally invertible!*

In particular

- $u(\Omega)$ is almost open;
- the composition $\mathbf{n} \circ u$ is measurable...
- ... and it does not depend on the representative of $\mathbf{n}$.

# Stabilty of the invertibility

**Lemma**

*Let $u, u_k \in \mathcal{W}(\Omega, \mathbb{R}^3)$ be such that $u_k \rightharpoonup u$ in $W^{1,3}$. Then $u_k$ converges to $u$ uniformly. Moreover, for any $x_0 \in \Omega_u$ there exist open neighborhoods $O, O_k \subset \Omega$ of $x_0$, $r = r(x_0) > 0$, and $w, w_k : B_r(y_0) \to \mathbb{R}^3$ with $y_0 = u(x_0)$ such that*

- $u(O) = B_r(y_0)$ *and* $w \circ u(x) = x$ *a.e.* $x \in O$;
- $u_k(O_k) = B_r(y_0)$ *and* $w_k \circ u_k(x) = x$ *a.e.* $x \in O_k$;
- $\nabla w(y) = (\nabla u)^{-1}(w(y))$ *a.e.* $y \in B_r(y_0)$;
- $\nabla w_k(y) = (\nabla u_k)^{-1}(w_k(y))$ *a.e.* $y \in B_r(y_0)$;
- $\chi_{O_k} \to \chi_O$ *pointwise a.e.*;
- $w, w_k \in W^{1,\frac{3}{2}}(B_r(y_0), \mathbb{R}^3)$ *and* $w_k \rightharpoonup w$ *in* $W^{1,\frac{3}{2}}$;
- $\mathrm{cof}\nabla w, \mathrm{cof}\nabla w_k \in L^3(B_r(y_0), \mathbb{R}^{3\times 3})$ *and* $\mathrm{cof}\nabla w_k \rightharpoonup \mathrm{cof}\nabla w$ *in* $L^3$.

In order to prove the last point, because of the low integrability of $\nabla w_k$, we cannot appeal to the usual continuity of the cofactor.

### Trick

*We use a pull-back.*

Remember that if $F \in \mathcal{M}$, then $\mathrm{cof}\, F^T = F^{-1}$. By a change of variables we have

$$\int_{B_r(y_0)} |\mathrm{cof} \nabla w_k|^3 dy = \int_{B_r(y_0)} |(\nabla w_k)^{-1}|^3 dy = \int_{O_k} |\nabla u_k|^3 dx.$$

Let $\phi \in C_0^\infty(B_r(y_0))$. Note that $\chi_{O_k}\phi \circ u_k$ converges to $\chi_O \phi \circ u$ pointwise a.e. and therefore in $L^p$.

$$\lim_k \int_{B_r(y_0)} \phi(y) \mathrm{cof} \nabla w_k(y) dy = \lim_k \int_{O_k} \phi(u_k(x))(\nabla u_k(x))^T dx$$
$$= \int_O \phi(u(x))(\nabla u(x))^T dx = \int_{B_r(y_0)} \phi(y) \mathrm{cof} \nabla w(y) dy.$$

# Main result

**Theorem**

*Assume that $\widetilde{W}$ satisfies the following coercivity condition:*

$$\widetilde{W}(F) \geq c_1|F|^3 - c_2 \quad \forall F \in \mathcal{M}.$$

*Given* $(u_0, \mathbf{n}_0) \in \mathcal{W}(\Omega, \mathbb{R}^3) \times H^1(u_0(\Omega), \mathbb{S}^2)$ *such that* $\mathcal{I}(u_0, \mathbf{n}_0)$ *is finite, define* $\mathcal{W}_{u_0}(\Omega, \mathbb{R}^3) := \{u \in \mathcal{W}(\Omega, \mathbb{R}^3) : u = u_0 \text{ on } \partial\Omega\}$. *Then, there exists* $(u, \mathbf{n}) \in \mathcal{W}_{u_0}(\Omega, \mathbb{R}^3) \times H^1(u(\Omega), \mathbb{S}^2)$ *minimizing* $\mathcal{I}$.

# Proof

Let $\{(u_k, \mathbf{n}_k)\} \subset \mathcal{W}_{u_0}(\Omega, \mathbb{R}^3) \times H^1(u_k(\Omega), \mathbb{S}^2)$ be a minimizing sequence. Let also $u \in \mathcal{W}_{u_0}(\Omega, \mathbb{R}^3)$ be the weak limit of $\{u_k\}$. By locality, there exists $\mathbf{n} \in H^1(u(\Omega), \mathbb{S}^2)$ s.t.

$$\lim_k \mathbf{n}_k = \mathbf{n} \ \text{ w*-}L^\infty \quad \text{and} \quad \lim_k \nabla \mathbf{n}_k = \nabla \mathbf{n} \ \text{ w-}L^2.$$

Why? Because when you fix a $y_0 \in u(\Omega)$ you can find $r$ and $\{O_k\} \subset \Omega$ such that $B_r(y_0) = u_k(O_k) \subset u_k(\Omega)$ for $k$ large enough.

Of course $\liminf_k \mathcal{I}_{\text{nem}}(u_k, \mathbf{n}_k) \geq \mathcal{I}_{\text{nem}}(u, \mathbf{n})$.

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It remains to show that $\liminf_k \mathcal{I}_{\mathrm{mec}}(u_k, \mathbf{n}_k) \geq \mathcal{I}_{\mathrm{mec}}(u, \mathbf{n})$.

## Trick

*We use a push-forward.*

$$\int_{O_k} W_{\mathrm{mec}}\big(\nabla u_k(x), \mathbf{n}_k(u_k(x))\big)\, dx = \int_{O_k} \widetilde{W}\big(V_{\mathbf{n}_k}^{-1}(u_k(x))\nabla u_k(x)\big)\, dx$$

$$= \int_{B_r(y_0)} \widetilde{W}\big(V_{\mathbf{n}_k}^{-1}(y)(\nabla w_k)^{-1}(y)\big)\, dy = \int_{B_r(y_0)} \widetilde{W}\big((\nabla w_k V_{\mathbf{n}_k})^{-1}(y)\big)\, dy$$

The point is that the functional is polyconvex also in the deformed configuration!

- $(\nabla w_k V_{\mathbf{n}_k})^{-1} = \mathrm{cof}(\nabla w_k V_{\mathbf{n}_k})^T$;
- $\mathrm{cof}(\nabla w_k V_{\mathbf{n}_k})^{-1} = (\nabla w_k V_{\mathbf{n}_k})^T$.

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The “perturbation” is not important.

Other (recent) works in this framework

- A Landau-De Gennes theory of liquid crystal elastomers. M. C. Calderer, C. G. Garzón & B. Yan. Preprint.

- Existence results for incompressible magnetoelasticity. M. Kružík, U. Stefanelli & J. Zeman Preprint.

Both with $u \in W^{1,p}$, $p > 3$.

# Open problems

- It should be desirable to extend the result to weaker coercivity assumptions already considered in nonlinear elasticity, such as

$$\widetilde{W}(F) \geq c_1|F|^2 + c_2|\mathrm{cof}\, F|^{3/2} - c_3.$$

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