Existence of solutions to models for nematic elastomers via lower semicontinuity in the deformed configurations

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Nematic elastomers are rubber-like materials constituted by a networks of cross-linked polymer chains in which are incorporated, or attached sideways, elongated rigid monomer units, called nematic mesogens. Their orientational order is described by a director field $n$. 
The coupling between nematic orientational order and rubber elasticity is the origin of a strong anisotropic behaviour: the alignment of nematic mesogens in a neighborhood of a point \( y \) with respect to a given configuration of the sample along an average direction \( n(y) \), induces a spontaneous distortion given by

\[
V_n := \alpha n \otimes n + \sqrt{\alpha} (I - n \otimes n).
\]

The tensor \( V_n \) represents a uniaxial stretch along the direction \( n \) of amplitude \( \alpha > 0 \).
Energy describing nematic elastomers

For nematic elastomers, DeSimone-Teresi have proposed the following variational nonlinear model:

\[
\mathcal{I}(u, n) := \int_{u(\Omega)} |\nabla n(y)|^2 dy + \int_{\Omega} \mathcal{W}_{\text{mec}}(\nabla u(x), n(u(x))) \, dx
\]

- \( u : \Omega \to \mathbb{R}^3 \) is a deformations of a body whose reference configuration is \( \Omega \subset \mathbb{R}^3 \);
- \( n : u(\Omega) \to S^2 \) is the director field describing the nematic order in the elastomer.
The mechanical response is governed by the coupling of rubber elasticity with the orientational order of the molecules.

\[ W_{\text{mec}}(F, n) := W(V_n^{-1} F), \]

where \( W : \{ F \in \mathbb{R}^{3 \times 3} : \det F = 1 \} \to [0, \infty) \) is a polyconvex energy and \( V_n \) is, as we said, the stretch in the direction \( n \in S^2 \) of a fixed amplitude \( \alpha > 0 \).
The Frank energy penalizes spatial variations of the nematic director.

The point is that when large deformations are in order, it is 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 director field is defined in the deformed configuration.*
- *We will also see a particular class of Sobolev maps in order to implement the previous solution.*
The difficulties here are that (1) our energy functional has two terms, the Frank one defined on the deformed configuration, and the mechanical one defined on the reference configuration, (2) there is a composition in the mechanical term...

We need to localize the first term and to push-forward the second one in order to work on the same domain, and to eliminate the composition. 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 $n \circ u$ is not measurable;
- $u_k \rightarrow u$ does not imply $\chi_{u_k}(\Omega) \rightarrow \chi_{u}(\Omega)$;
- $u_k \rightarrow u$ and $n_k \rightarrow n$ do not imply $n_k \circ u_k \rightarrow n \circ u$. 

Ambient space of our problem

The easy one: 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 (pure math!)

\begin{itemize}
  \item \( u(\Omega) \) is almost open;
  \item the composition \( n \circ u \) is measurable;
  \item \( \ldots \) and it does not depend on the representative of \( n \).
\end{itemize}
Stability 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 \( x_0 \in \Omega \) there exist open neighborhoods \( O, O_k \subset \Omega \) of \( x_0 \), \( r = r(x_0) > 0 \), and \( w, w_k : B_r(y_0) \rightarrow \mathbb{R}^3 \) 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. \( y \in B_r(y_0) \);
- \( \chi_{O_k} \rightarrow \chi_O \) 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 \( W^{1,\frac{3}{2}} \);
- \( \text{cof } \nabla w, \text{cof } \nabla w_k \in L^3(B_r(y_0), \mathbb{R}^{3 \times 3}) \) and \( \text{cof } \nabla w_k \rightharpoonup \text{cof } \nabla w \) in \( L^3 \).
In order to prove this 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 $\text{cof } F^T = F^{-1}$. By a change of variables we have

$$\int_{B_r(y_0)} \left| \text{cof } \nabla w_k \right|^3 dy = \int_{B_r(y_0)} \left| (\nabla w_k)^{-1} \right|^3 dy = \int_{O_k} \left| \nabla u_k \right|^3 dx.$$
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 $L^p$.

$$\lim_k \int_{B_r(y_0)} \phi(y) \text{cof} \nabla w_k(y) dy = \lim_k \int_{O_k} \phi(u_k(x))(\nabla u_k(x))^T dx$$

$$= \int_{O} \phi(u(x))(\nabla u(x))^T dx = \int_{B_r(y_0)} \phi(y) \text{cof} \nabla w(y) dy.$$
Existence result

**Theorem**

Assume that $W$ satisfies the following coercivity condition:

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

Given $(u_0, n_0) \in \mathcal{W}(\Omega, \mathbb{R}^3) \times H^1(u_0(\Omega), S^2)$ such that $I(u_0, n_0)$ 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 $(u, n) \in \mathcal{W}_{u_0}(\Omega, \mathbb{R}^3) \times H^1(u(\Omega), S^2)$ minimizing $I$. 
Proof

Let \( \{(u_k, n_k)\} \subset \mathcal{W}_{u_0}(\Omega, \mathbb{R}^3) \times H^1(u_k(\Omega), \mathbb{S}^2) \) 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 \( n \in H^1(u(\Omega), \mathbb{S}^2) \) s.t.

\[
\lim_{k} n_k = n \quad \text{w}^*-L^\infty \quad \text{and} \quad \lim_{k} \nabla n_k = \nabla n \quad \text{w}-L^2.
\]

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 \( \liminf_{k} I_{\text{nem}}(u_k, n_k) \geq I_{\text{nem}}(u, n) \).
Proof

Let \( \{(u_k, n_k)\} \subset \mathcal{W}_{u_0}(\Omega, \mathbb{R}^3) \times H^1(u_k(\Omega), \mathbb{S}^2) \) 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 \( n \in H^1(u(\Omega), \mathbb{S}^2) \) s.t.

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Of course \( \liminf_k \mathcal{I}_{\text{nem}}(u_k, n_k) \geq \mathcal{I}_{\text{nem}}(u, n) \).
It remains to show that \( \liminf_k I_{\text{mec}}(u_k, n_k) \geq I_{\text{mec}}(u, n) \).

**Trick**

*We use a push-forward.*

\[
\int_{O_k} W_{\text{mec}}\left(\nabla u_k(x), n_k(u_k(x))\right) \, dx = \int_{O_k} W\left(V_{n_k}^{-1}(u_k(x))\nabla u_k(x)\right) \, dx \\
= \int_{B_r(y_0)} W\left(V_{n_k}^{-1}(y)(\nabla w_k)^{-1}(y)\right) \, dy = \int_{B_r(y_0)} W\left((\nabla w_k V_{n_k})^{-1}(y)\right) \, dy
\]
The point is that the functional is polyconvex also in the deformed configuration!

\[ (\nabla w_k V_{n_k})^{-1} = \text{cof}(\nabla w_k V_{n_k})^T; \]

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The “perturbation” is not important.
Possible improvement: it should be desirable to set up the problem in a larger space in order to allow less regular deformations.

We define a suitable subclass of deformations in $W^{1,p}$, $p > n - 1$, that are regular enough (no cavitations).

At the moment deformations with cavitations seem forbidding. However, It would also be interesting to formulate a model that allows for cavitations, through a functional that measures in the deformed configuration the surface area of the cavities opened by the deformation.
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Ingredients required

- $u(\Omega)$ is “open”;
- $u$ is locally invertible with Sobolev inverse;
- some stability.
A suitable class

Definition

The class $\mathcal{A}_p$ is constituted by the maps $u \in W^{1,p}(\Omega, \mathbb{R}^n)$ satisfying $\det Du \in L^1_{\text{loc}}(\Omega)$, $\mathcal{E}(u) = 0$ and $\det Du > 0$ a.e.

The condition $\mathcal{E}(u) = 0$ is satisfied for instance when $\text{cof } \nabla u \in L^{\frac{n}{n-1}}(\Omega, \mathbb{R}^{n \times n})$. 
Damage

**Definition**

We define the *topological image* of a point \( x \in \Omega \)

\[
\text{im}_T(u, x) = \bigcap_{r: B(x, r) \text{ good}} \text{im}_T(u, B(x, r)),
\]

and \( NC := \{ x \in \Omega : \mathcal{H}^0(\text{im}_T(u, x)) > 1 \} \).

From the physical point of view, when \( x \in NC \) we interpret \( \text{im}_T(u, x) \) as a **damage zone**. The set \( NC \) is less than \( \mathcal{H}^1 \)-negligible, while the damage zone is negligible. The function \( u \) is continuous outside \( NC \).
Proposition

The map $u$ is almost locally invertible and its inverse is Sobolev. The stability still works.

The set where we have loss of injectivity is negligible and it is squeezed in a $\mathcal{H}^{n-1}$-negligible set. We interpret its image as a degeneration of the material due to extreme compression.