Injective elastic deformations via vanishing self-repulsion

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Outline

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Elasticity: some basics

Global invertibility as a constraint: The Ciarlet-Nečas condition and associated penalization terms

Injectivity via self-replusion in nonlinear elasticity

Numerical experiments

Summary

Variational Nonlinear Elasticity: the basic model

Laws

Observable deformations y^* (locally) **minimize**

$$E(y) := E^{el}(y) + E^{ext}(y).$$

States (unknowns)

$\boldsymbol{y : \Omega \to \mathbb{R}^d}$, the "**deformation**" of the elastic body (e.g. $\boldsymbol{d = 3}$);
$\nabla y : \Omega \to \mathbb{R}^{d\times d}$ denotes its "**deformation gradient**"

Data

- $\boldsymbol{\Omega} \subset \mathbb{R}^d$ bounded domain, the "**reference configuration**"
- $\boldsymbol{W} : \mathbb{R}^{d\times d} \to [0, +\infty]$, which allows us to calculate the "**elastic energy**" $\boldsymbol{E^{el}(y) := \int_\Omega W(\nabla y(x))\, dx}$
- (conservative) external forces and their potential $\boldsymbol{E^{ext}(y)}$
- (optional) boundary conditions for y

Variational NLE: the basic model

Minimize

$$E(y) := E^{el}(y) + E^{ext}(y), \quad E^{el}(y) := \int_\Omega W(\nabla y(x))\, dx.$$

Typical assumptions on W, for all $F \in \mathbb{R}^{d\times d}$

- (**frame indifference**) $W(QF) = W(F) \quad \forall\, Q \in SO(d)$
- (**orientation preserving**) $W(F) = +\infty$ iff $\det F \leq 0$.
- W is continuous, **penalizes large strain and compression**:

  $$W(F) \geq c\,|F|^p + c\,|\det F|^{-r} - C,$$

  with constants $c, C > 0$, $\boldsymbol{p > d}$, $r > 0$.
- W is **polyconvex**, e.g., if $d = 3$,
  $W(F) = h(F, \operatorname{cof} F, \det F)$ with a convex function h.

Variational NLE: A few known results

Minimize

$$E(y) := E^{el}(y) + E^{ext}(y), \quad E^{el}(y) := \int_\Omega W(\nabla y(x))\, dx.$$

Existence of minimizers

If (*) holds, $\partial\Omega$ is Lipschitz, and E^{ext} and the boundary conditions imposed on y are reasonable:

- E has a global minimizer in $y^* \in W^{1,p}$ (Ball 1977).

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On local invertibility

For all deformations y with finite energy:

- $\det \nabla y > 0$ a.e. in Ω and $y \in C^0(\bar{\Omega}; \mathbb{R}^d)$
- Around a.e. $x \in \Omega$, y is a.e. locally invertible (Fonseca&Gangbo 1995)

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- Everywhere local invertibility and uniform lower bound on $\det \nabla y$ for some non-simple materials (suitable higher order regularization) (Healey&K. 2009)

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- Everywhere local invertibility and uniform lower bound on $\det \nabla y$ for some non-simple materials (suitable higher order regularization) (Healey&K. 2009)
- Additional local properties **if the energy sufficiently controls the distortion** of ∇y: openness and discreteness (Villamor&Manfredi 1998; Hencl&Koskela 2014)

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Lavrentiev phenomenon

- A **Lavrentiev phenomenon** is possible: $\inf_{y \in W^{1,\infty}} E(y) > \min_{y \in W^{1,p}} E(y)$ for a particular example (Foss&Hrusa&Mizel 2003).
  In particular, discretizations with piecewise affine elements can fail to converge!
- (In principle) avoidable numerically by using non-conforming elements (Negrón Marrero 1990): Use (y, F) instead of $(y, \nabla y)$ while penalizing the difference. The "good" scaling regime for the penalization versus the grid size is not explicitly known though!

Variational NLE: Global invertibility from the boundary

Minimize

$$E(y) := E^{el}(y) + E^{ext}(y), \quad E^{el}(y) := \int_\Omega W(x, \nabla y(x))\, dx.$$

Global invertibility for orientation preserving maps

- Global invertibility (a.e.) can be added as a constraint, the Ciarlet-Nečas condition (CNc)

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Moreover, for all $y \in W^{1,p}_+$ ("+": $\det \nabla y > 0$ a.e.), $p > d$:

- If $y = \hat{y}$ on $\partial\Omega$ for a globally invertible $\hat{y} \in C^0(\bar{\Omega}; \mathbb{R}^d)$, (i.e., $y|_{\partial\Omega}$ admits a homeomorphic extension) then y is a.e. globally invertible (Ball 1981).
  (Less regularity: Henao&Mora-Corral&Oliva 2021)

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- If $y|_{\partial\Omega}$ is invertible or can be uniformly approximated by such maps ("$y \in \mathrm{AIB}$") and **Ω is "without holes"**, then y is a.e. globally invertible (K. 2020).

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The Ciarlet-Nečas condition (CNc) in a discrete setting?

- **No computationally feasible projection onto (CNc) is known**
  (Partial results for C^0-elements: [Aigerman&Lipman 2013])
  Without projection, (CNc) cannot be used as a discrete constraint!

$$\text{(CNc)} \quad \int_\Omega |\det \nabla y(x)| \, dx \le |y(\Omega)| \quad (\Longleftrightarrow y \text{ a.e. injective})$$

The Ciarlet-Nečas condition and numerics?

(CNc) as a "soft" constraint, via (nonlocal) **penalty term**?

- [Mielke&Roubíček 2016] (e.g.):

$$E_\varepsilon^{\text{CN-MR}}(y) := \frac{1}{\varepsilon}\left(\int_\Omega |\det \nabla y(x)|\, dx - |y(\Omega)|\right)$$

  Rigorously reproduces (CNc), but not a standard integral functional. Hard to implement. Expensive and non-smooth. No surface variant known. Contact relaxes to interpenetration.

- [Bartels&Reiter 2018], [Yu&Brakensiek& Schumacher&Crane 2021], etc.: Nonlocal geometric energies (tangent point, Möbius, etc.). Relatively cheap. Singular, not "lower order", force high regularity. Lavrentiev phenomenon?

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The Ciarlet-Nečas condition and numerics?

(CNc) as a "soft" constraint, via (nonlocal) **penalty term**?

- [K.&Valdman 2020]: Lower order double integral term. Expensive, because (theoretically) active on all of $\Omega \times \Omega$. Known to rigorously reproduce (CNc) only if deformations are at least locally bi-Lipschitz. Lavrentiev phenomenon otherwise? Rigorous for higher gradient nonlinear elasticity.

$$\text{(CNc)} \quad \int_\Omega |\det \nabla y(x)| \, dx \leq |y(\Omega)| \quad (\Longleftrightarrow y \text{ a.e. injective})$$

Towards other penalization terms

Aim

Find other penalty terms $E_\varepsilon^{CN}(y)$ realizing (CNc) as a limit.

Must have for all admissible y:

- $$\Gamma - \lim_{\varepsilon \to 0} E_\varepsilon^{CN}(y) = \begin{cases} 0 & \text{if and only if } y \text{ satisfies (CNc),} \\ +\infty & \text{otherwise} \end{cases}$$

Nice to have as well:

- $E_\varepsilon^{CN}(y)$ is easier and **cheaper** to compute. **Have E_ε^{CN} only act on (or near) $\partial\Omega$.**
- $E_\varepsilon^{CN}(y)$ allows smooth version
- $E_\varepsilon^{CN}(y) \implies y$ globally invertible (even for finite $\varepsilon > 0$!)
- adding E_ε^{CN} does not create additional stable states (?)

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Nonlinear elasticity with controlled distortion

We now consider the nonlinear elastic energy

$$E^{el}(y) = \int_\Omega W(\nabla y)\, dx \quad \text{with (e.g.)} \quad W(F) := |F|^p + \frac{1}{(\det F)^r}$$

with $\boldsymbol{p > d}$ **and** $\boldsymbol{r > 0}$ **big enough** so that for some $\boldsymbol{\gamma > d-1}$,

$$(K^O(F))^\gamma := \left(\frac{|F|^d}{\det F}\right)^\gamma \leq C\, W(F) \quad \text{for all } F \in GL_d^+.$$

Consequences of this **control of** $\boldsymbol{K^O(\nabla y)}$ by $E^{el}(y)$:

Theorem (Villamor&Manfredi 1998)

Let $y \in W_+^{1,p}(\Omega;\mathbb{R}^d)$, $p > d$. If $K^O(\nabla y) \in L^\gamma(\Omega)$ for a $\gamma > d-1$, then y is **open** and discrete.

Nonlinear elasticity with controlled distortion

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Consequences of this **control of** $\boldsymbol{K^O(\nabla y)}$ by $E^{el}(y)$:

Lemma (Grandi&Kružík&Mainini&Stefanelli 2019)

Let $y \in W_+^{1,p}(\Omega;\mathbb{R}^d)$, $p > d$, be an **open** map satisfying (CNc).
Then $\boldsymbol{y}$ **is a homeomorphism** on Ω.

'Inverse Sobolev–Slobodeckiĭ' self-repulsion

A new self-repulsion term, with parameters $0 \leq s < 1$, $q \geq 1$:

$$\mathcal{D}_\delta(y) := \int_{U_\delta} \int_{U_\delta} \frac{|x - \tilde{x}|^q}{|y(x) - y(\tilde{x})|^{d+sq}} |\det \nabla y(x)| \, |\det \nabla y(\tilde{x})| \; dx \, d\tilde{x}$$

where $\delta > 0$ and $U_\delta \subset \Omega$ is an open δ-neighborhood of $\partial\Omega$ in Ω:

$$\{x \in \Omega \mid \operatorname{dist}(x; \partial\Omega) < \tfrac{\delta}{2}\} \subset U_\delta$$

Remark (inverse (s, q)-Sobolev-Slobodeckiĭ seminnorm)

If y is a.e.-invertible, a change of variables gives

$$\mathcal{D}_\delta(y) = \int_{y(U_\delta)} \int_{y(U_\delta)} \frac{\left|y^{-1}(z) - y^{-1}(\tilde{z})\right|^q}{|z - \tilde{z}|^{d+sq}} \, dz \, d\tilde{z}$$

This is the (s, q)-Sobolev-Slobodeckiĭ seminnorm of y^{-1} on $y(U_\delta)$.

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Proposition (K.& Reiter 2022)

$\mathcal{D}_\delta$ is weakly lower semicontinuous in $W^{1,p}_+$.

Proof: Essentially exploit "separate polyconvexity" for the double integral: Combine the weak continuity of the determinant with separate convexity of the integrant in each of the two determinants (cf. ELBAU 2011 for the role of separate convexity).

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Proposition (perfect self-repulsion, K.& Reiter 2022)

If y is an open map and $sq \geq 0$, $\mathcal{D}_\delta(y) < \infty$ implies (Cnc) on U_δ.

Proof: By contradiction; essentially a simple estimate exploiting the singular denominator of $\mathcal{D}$.

Energy convergence for vanishing self-repulsion

$$E_{\varepsilon,\delta}(y) := \begin{cases} E^{el}(y) + \varepsilon \mathcal{D}_\delta(y) & \text{if } y \in W^{1,p}_+(\Omega, \mathbb{R}^d), \\ +\infty & \text{else.} \end{cases}$$

$$E_0(y) := \begin{cases} E^{el}(y) & \text{if } y \in W^{1,p}_+(\Omega, \mathbb{R}^d) \text{ satisfies (CNc)}, \\ +\infty & \text{else.} \end{cases}$$

Theorem 3 (K.&Reiter 2022)

Suppose that $p > d$, $0 \le s < 1$, $q \ge 1$, Ω is a Lipschitz **domain "without holes"**, $\boldsymbol{E^{el}}$ **controls the distortion** as before and

$$s - \frac{d}{q} \le 1 - \frac{d}{\sigma}, \quad \text{where } \sigma := \frac{(r+1)p}{r(d-1)+p} (> d).$$

Then $\boldsymbol{E_{\varepsilon,\delta}}$ **Gamma-converges to** $\boldsymbol{E_0}$ in the weak topology of $W^{1,p}$, as $(\varepsilon, \delta) \to (0,0)$ (the scaling regime can be arbitrary!).

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Remark (on σ and the assumed inequality)

The assumption

$$s - \frac{d}{q} \leq 1 - \frac{d}{\sigma}, \quad \text{where } \sigma := \frac{(r+1)p}{r(d-1)+p} (> d),$$

is used for an embedding and implies that

$$\mathcal{D}_U(y) \leq C \left\| y^{-1} \right\|_{W^{1,\sigma}(y(U))}$$

if y is invertible and $y(U)$ has Lipschitz boundary.

Energy convergence for vanishing self-repulsion

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Remark (recovery by homeomorphisms)

As constructed in the proof, recovery sequences consist of homeomorphisms on $\overline{\Omega}$ with inverse in $W^{1,\sigma}$ which converge strongly in $W^{1,p}$.

Convergence of energies: elements of the proof

Crucial tools for the construction of the recovery sequence:

Lemma (domain shrinking)

Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain. Then there exists a sequence of C^∞-diffeomorphisms

$$\Psi_j : \overline{\Omega} \to \Psi_j(\overline{\Omega}) \subset\subset \Omega$$

such that for all $m \in \mathbb{N}$,

$$\Psi_j \underset{j\to\infty}{\longrightarrow} \mathrm{id} \quad \text{in } C^m(\overline{\Omega}; \mathbb{R}^d).$$

Lemma (composition with domain shrinking is continuous)

For each $f \in W^{k,r}(\Omega; \mathbb{R}^m)$, $k \in \mathbb{N}_0$, $1 \leq r < \infty$, $m \in \mathbb{N}$,

$$f \circ \Psi_j \to f \quad \text{in } W^{k,r}(\Omega; \mathbb{R}^m).$$

Outline

Numerical experiments: symmetric (J. Valdman)

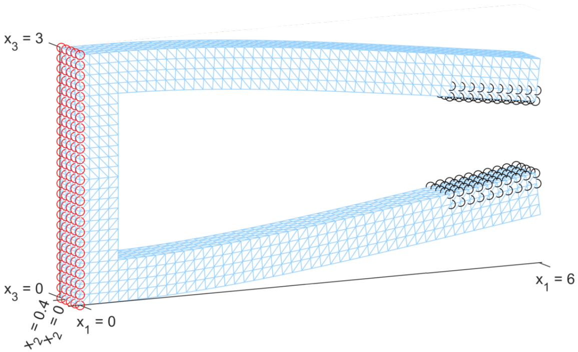

Figure : Initial deformed mesh with red Dirichlet and black possible non-penetration nodes.

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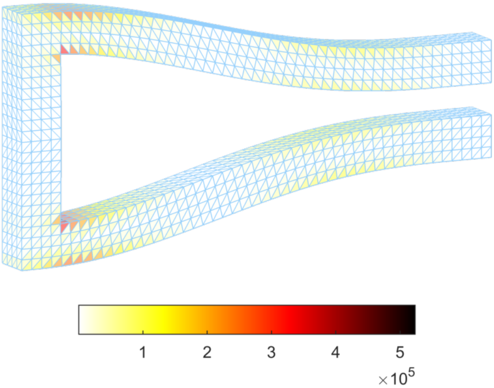


Figure : Deformed mesh with the underlying linear elasticity density.

Numerical experiment: symmetric (J. Valdman)

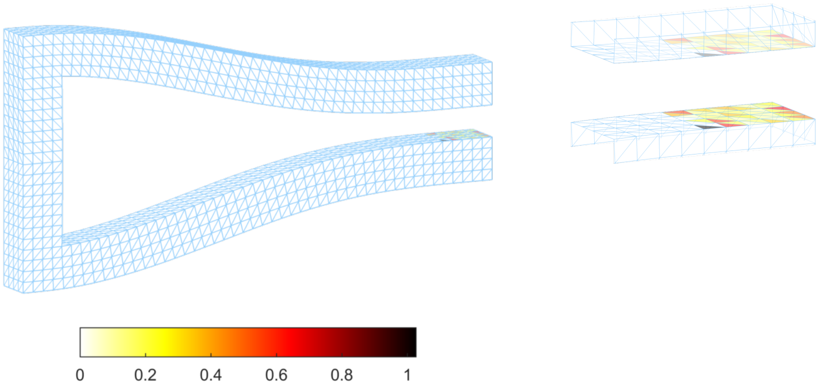
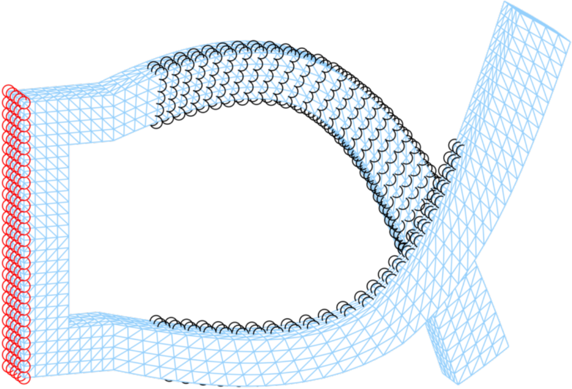


Figure : Deformed mesh with the underlying non-penetration density (left) and its magnified part (right).

Numerical experiment 2: asymmetric (J. Valdman)



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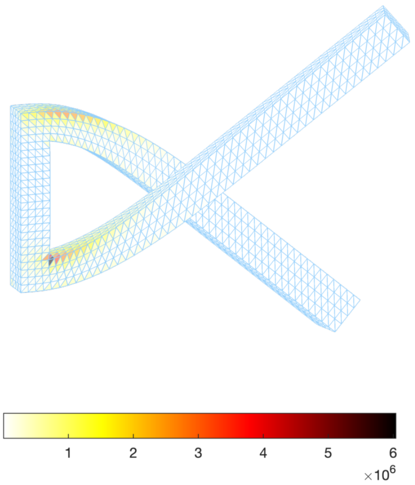

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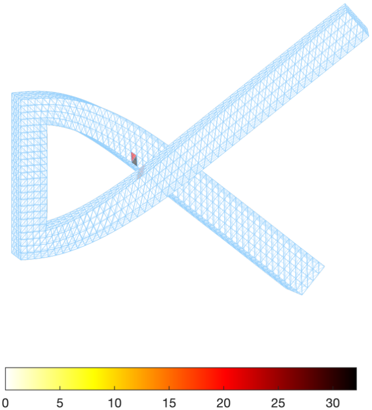

Figure : Deformed mesh with the underlying non-penetration density

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The end: summary and remarks

For (Cnc), we have new penalty terms, acting only on or near the boundary, with self-repulsive effect.

- They are **proven to reproduce (CNc)** in the following cases:
  - (i) linear elasticity, given a local bi-Lipschitz constraint [K.&Valdman, work in progress] (not discussed in detail here)
  - (ii) standard nonlinear elasticity, if there is enough energetic control of the distortion (to obtain openness and discreteness) [K.&Reiter 2022].
- They are much cheaper to evaluate numerically, especially if paired with linear elasticity
- They automatically lead to **approximation by homeomorphisms** on $\overline{\Omega}$
- Extensions: $\mathcal{D}_\delta$ also has a surface variant