

Problems in Pattern Formation, Geometry and Design of Materials

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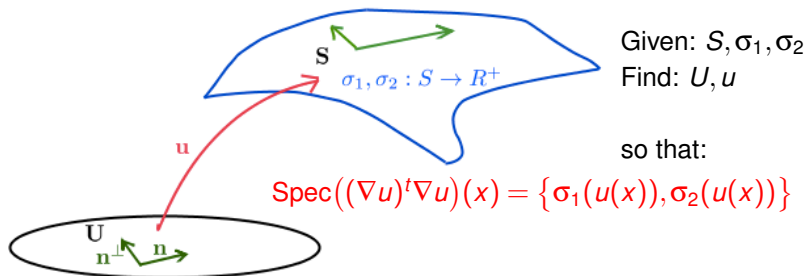
University of Pittsburgh

NSF-SIAM Symposium on Mathematical
and Computational Aspects of Materials Science

– 14 March, 2015 –

- Manipulating the micro-structure of material \implies desired change in its mechanical responses.
 - Actuation of thin nematic glass sheets
 - Halftone gel lithography
 - Understanding morphogenesis in response to inhomogeneous and incompatible prestrain
 - Pattern formation: wrinkling / blistering / crumpling ...
- Mathematical problems combining geometry, analysis, calculus of variations, pdes, related to practical questions of material design.
 - Forward and inverse problems of isometric immersions
 - Energy scaling laws
 - Incompatible elasticity / dimension reduction
 - Questions of regularity / uniqueness / existence of solutions to nonconvex problems

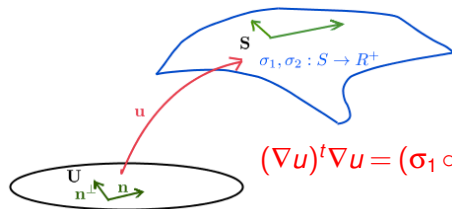
Geometric design problem in actuation of liquid crystals



- Find eigenvectors $\vec{n}(x), \vec{n}^\perp(x)$ of $(\nabla u)^t \nabla u$
- Align the liquid crystal director in the flat configuration with $\vec{n}(x)$
- Spontaneous actuation of the metric G will result in manufacturing surface S :

$$(\nabla u)^t \nabla u = (\sigma_1 \circ u) \vec{n} \otimes \vec{n} + (\sigma_2 \circ u) \vec{n}^\perp \otimes \vec{n}^\perp = G$$

Geometric design problem in actuation of liquid crystals

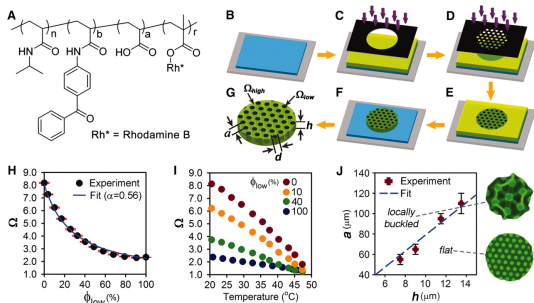


May not yield S !

$$(\nabla u)^t \nabla u = (\sigma_1 \circ u) \vec{n} \otimes \vec{n} + (\sigma_2 \circ u) \vec{n}^\perp \otimes \vec{n}^\perp = G$$

- Among $y : U \rightarrow \mathbb{R}^3$ satisfying $(\nabla y)^t \nabla y = G$, the energy minimizing y will be realised: $E(y) = \int_U |H_y|^2 \equiv \int_U |I_y|^2$
- Another problem (more restrictive):
Given $g : S \rightarrow \mathbb{R}_{sym, pos}^{2 \times 2}$ prestrain metric on S
Find $u : U \rightarrow S$ such that $(\nabla u)^t \nabla u = g \circ u = G$
- Energy minimization criterion as before. [Acharya-L-Pakzad'14]

Half-tone gel lithography



[Kim, Hanna, Byun, Santangelo, Hayward – Science, 2012]

- Method of photopatterning polymer films that yields temperature-responsive gel sheets that can transform between a flat state and a prescribed 3d shape
- Lightly cross-linked dots embedded in a cross-linked matrix \implies “nearly continuous” 2d “patterns of swelling” (prestrain metric G)

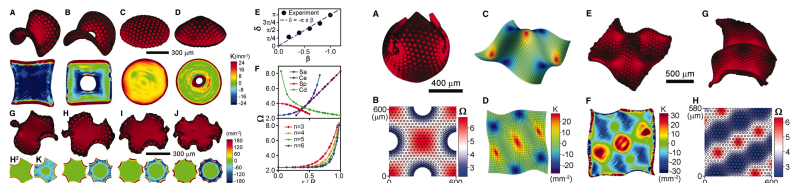
Half-tone gel lithography

- **Forward problem:**

Given G on U , minimize: $E^h(y) = h^2 \int_U |I|_y|^2 + \int_U |I_y - G|^2$

- Euler-Lagrange equations given in terms of $I = I_y$ and $II = I|_y$:

$$(*) \quad \begin{cases} F(I, II; G) = 0 \\ \text{compatibility conditions via Gauss-Codazzi eqns} \\ \text{boundary conditions} \end{cases}$$



[Kim, Hanna, Byun, Santangelo, Hayward – Science, 2012]

- **Inverse design problem:** [Dias, Hanna, Santangelo – Phys. Rev E, 2011]

Given S with parametrisation $u : U \rightarrow S$, yielding: $I = I_u$, $II = II_u$

Solve $(*)$ for $G \implies$ imprint $G \implies$ activate for S

General set-up: Incompatible elasticity

$$E(u) = \int_{\Omega} W(\nabla u \sqrt{G}^{-1}) dx, \quad u: \mathbb{R}^3 \supset \Omega \rightarrow \mathbb{R}^3$$

- $E(u) = 0$ if and only if: $(\nabla u)^t \nabla u = G$ and $\det \nabla u > 0$
- $Riem(G) \neq 0 \implies \inf_{u \in W^{1,2}(\Omega, \mathbb{R}^3)} E(u) > 0$

- Dimension reduction for prestrained thin films:

$$\Omega^h = U \times \left(-\frac{h}{2}, \frac{h}{2}\right), \quad E^h(u^h) = \frac{1}{h} \int_{\Omega^h} W(\nabla u \sqrt{G}^{-1}), \quad G(x', x_3) = G(x')$$

Questions: 1. Scaling: $\inf E^h \sim h^\beta$, 2. Asymptotics: $\operatorname{argmin} E^h$ as $h \rightarrow 0$

- Small energy theories $\beta \geq 2 \implies$ only 2 residual theories!

Theorem (L, Pakzad'09; Bhattacharya, L, Schaffner'14)

$\beta = 2$. Only valid when: $\exists y \in W^{2,2}(U, \mathbb{R}^3)$ $(\nabla y)^t \nabla y = G_{tan}$.
Then: $\operatorname{argmin} E^h \rightarrow \operatorname{argmin} I_2(y) = \int_U |\operatorname{sym}((\nabla y)^t \nabla \vec{b})|^2$.

Theorem (L, Raoult, Ricciotti'15)

$\beta = 4$. Only valid when: $R_{1212} = R_{1213} = R_{1223}(G) = 0$.
 $\operatorname{argmin} E^h \rightarrow \operatorname{argmin} I_4 = \int_U |\operatorname{stretching}|^2 + |\operatorname{bending}|^2 + \int_U |Riem(G)|^2$.

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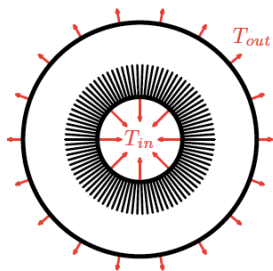
- Questions:



- Uniqueness / multiplicity of minimizers to I_2
- Uniqueness / multiplicity of minimizers to the “linearized problem”:
 $I_{2,lin}(v) = \int_U |\nabla^2 v|^2$; $\det \nabla^2 v = \text{curl}^t \text{curl } G_{tan}$
- Differences for positive / negative curvature of G_{tan}
- Geometry enters in a subtle manner; regularity questions for isometric immersions

[Klein, Efrati, Sharon - Science '07]

- In lower energy regimes, the minimizing sequences develop oscillatory behaviour \implies energy relaxation
- Energy comparison methods \implies certain patterns are energetically preferable
- **Example: Wrinkles of annular sheet loaded in the radial direction**
[Kohn, Bella – CPAM, 2014]

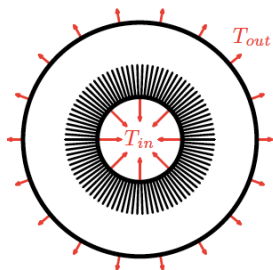


$$E^h(u^h) = \frac{1}{h} \int_{\Omega^h} W(\nabla u^h) + \left(\frac{T_{in}}{h} \int_{|x|=r} u \cdot \frac{x}{r} - \frac{T_{out}}{h} \int_{|x|=R} u \cdot \frac{x}{R} \right)$$

Then: $|\min_{u^h \in W^{1,2}} E^h - \min E_0| = O(h)$

where $E_0 =$ relaxation obtained by quasi-convexification + boundary terms

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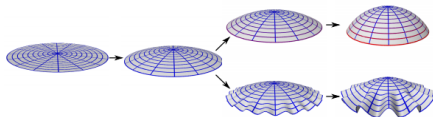


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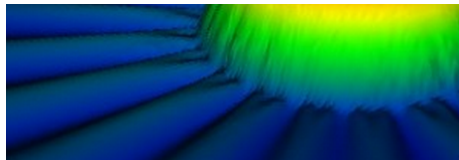
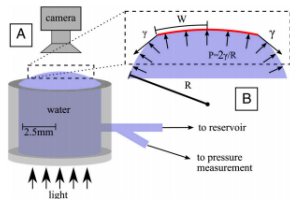
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- Lower bound estimates: $\min E^h - \min E_0 \geq ch$
- Upper bound construction of u^h , informed by experimental ansatz

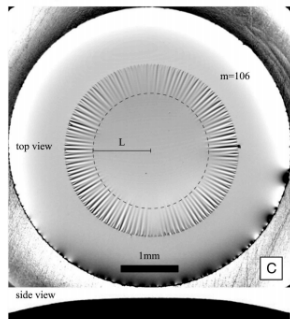


Wrinkling/ blistering/ crumpling ...

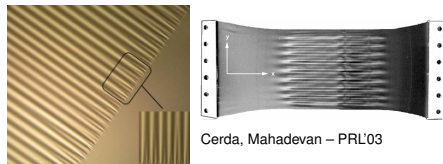


[Davidovitch et al, 2012]

- Wrinkle to crumple transition
- Smooth cascades
- Other patterns



[King, Schroll, Davidovitch, Menon - PNAS'12]



Cerda, Mahadevan – PRL'03

[Huang, Davidovitch, Santangelo, Russell, Menon – PRL'10]

Rigidity and flexibility

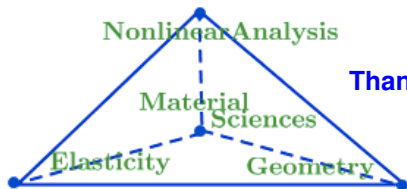
- Oscillatory behaviour \implies lower regularity in the limit \implies analytical difficulties (low regularity maps are “flexible”)

Theorem (Nash, Kuiper – 1955. **Convex integration for isom. immer.**)

Let G be a C^2 metric. Then its C^1 isometric immersions are dense (w.r.t C^0 norm) in the set of all short immersions of G .

Theorem (L-Pakzad – 2015. **Convex integration for Monge-Ampère**)

Let f be Hölder continuous. Then $C^{1,\alpha}$ solutions (for any $\alpha < \frac{1}{7}$) to $\det \nabla^2 v = f$ are dense in $C^0(U)$.



Thank you for your attention