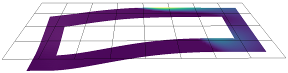
Simulation of Free Boundary Problems in the Nonlinear Bending of Elastic Rods and Plates



Sören Bartels

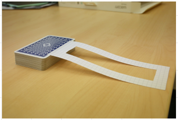
University of Freiburg, Germany

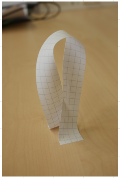
Berlin (online), September 15, 2021

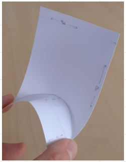
15th International Conference on Free Boundary Problems

Outline

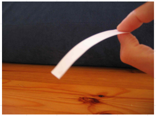
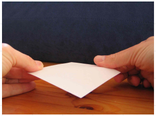
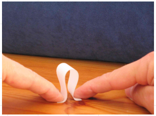
1. **Mathematical description**
2. **Numerical approximation**
3. **Model extensions**
4. **Summary**







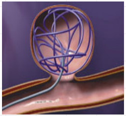
Nonlinear bending: Large deformations, incompressibility, nonuniqueness

Applications: Flexible bio structures, origami folding, aneurysm coiling

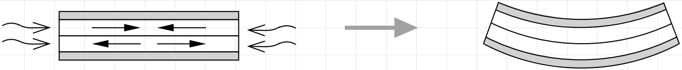

Source: www.sciencemag.org


Source: www.peakpx.com


Source: Uni Innsbruck

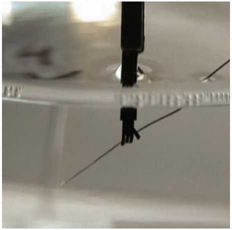
Goals: Modeling, simulation, optimization

Bilayers: Externally controlled large deformations



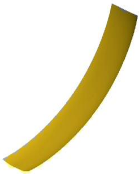
Application: Development of small scale technologies

[Smela et al. '95]



External Link

[B., Bonito & Nochetto '17]



External Link

Effects: Obstacles, self-contact

Mathematical description

Classical: Insert *ansatz* into 3D elastic model

Modern approach: Rigorous reduction from 3D with minimal assumptions

3D Hyperelasticity: Energy functional for deformation $y : \Omega \to \mathbb{R}^3$

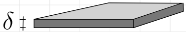
$$I^{3d}[y] = \int_\Omega W(\nabla y)\,\mathrm{d}x - \int_\Omega f \cdot y\,\mathrm{d}x$$

with isotropic stored energy density $W : \mathbb{R}^{3\times 3} \to \mathbb{R}_{\geq 0}$

$$W(\mathbb{I}_{3\times 3}) = 0, \quad W(QFR) = W(F) \quad \forall Q, R \in SO(3)$$

Bending: Determined for thin plate $\Omega_\delta = \omega \times (-\delta/2, \delta/2)$ via scaling

$$\min_{y \in \mathcal{A}} I^{3d}[y] \sim \delta^3$$



Γ-limit: [DeGiorgi '75] Identify functional I^{2d} such that

$$\lim_{\delta \to 0} \delta^{-3} I^{3d} = I^{2d}$$

Quantitative version of Liouville's theorem or nonlinear Korn inequality:

Lemma [Friesecke, James, Müller '01] For all $y \in W^{1,2}(\Omega_1;\mathbb{R}^3)$

$$\min_{R\in SO(3)} \|\nabla y - R\| \le C\big\|\mathrm{dist}(\nabla y, SO(3))\big\|.$$

Theorem [Kirchhoff 1850, FJM '01]. Functionals $\delta^{-3} I^{3d}$ Γ-converge to

$$I^{2d}[y] = \frac{\alpha}{2}\int_\omega |II|^2 \,\mathrm{d}x' - \int_\omega \widetilde{f}\cdot y \,\mathrm{d}x'$$

for isometries $y:\omega\to\mathbb{R}^3$, i.e., $I = \mathbb{I}_{2\times 2}$, with fundamental forms

$$I = \nabla y^{\mathsf{T}} \nabla y, \qquad II = \nu^{\mathsf{T}} D^2 y$$

and normal $\nu = \partial_1 y \times \partial_2 y$. Moreover, $I^{2d} = \infty$ otherwise.

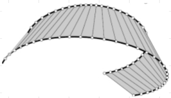
- fourth order, pointwise constraint, no injectivity
- attainment via $\widetilde{y}(x) = y(x') + \delta x_3 \nu(x') + \delta^2 (x_3^2/2) d(x')$
- extreme case - combined models involving δ, hierarchies, expansions?

Partial derivatives of C^2 isometry $y : \omega \to \mathbb{R}^3$ orthonormal

$$|\partial_1 y|^2 = 1, \quad |\partial_2 y|^2 = 1, \quad \partial_1 y \cdot \partial_2 y = 0$$

Implies $\partial_j^2 y \cdot \partial_k y = 0$ and

$$|II|^2 = 4H^2 = |\Delta y|^2 = |D^2 y|^2$$



- Gaussian curvature vanishes *(theorema egregium)*, developable surface
- cannot deform egg surfaces isometrically [Herglotz '43]
- same assertions for $W^{2,2}$ isometries [Pakzad '04, Hornung '08]

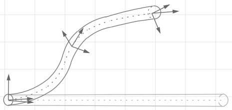
Model problem: Find $y : \omega \to \mathbb{R}^3$ minimal for

$$I^{2d}[y] = \frac{\alpha}{2} \int_\omega |D^2 y|^2 \,\mathrm{d}x' - \int_\omega \widetilde{f} \cdot y \,\mathrm{d}x'$$

subject to pointwise isometry constraint and clamped boundary conditions

$$\nabla y^{\mathsf{T}} \nabla y = \mathbb{I}_{2\times 2} \quad \text{and} \quad y|_{\gamma_D} = y_D, \; \nabla y|_{\gamma_D} = \phi_D$$

Consider elastic object with
circular cross-sections $\Omega_\delta = (0, L) \times B_\delta(0)$



Theorem [Mora & Müller '03] Limiting energy for $\delta \to 0$ given by

$$I[u, b, d] = \frac{c_b}{2} \int_0^L |u''|^2 \,\mathrm{d}x_1 + \frac{c_t}{2} \int_0^L (b' \cdot d)^2 \,\mathrm{d}x_1$$

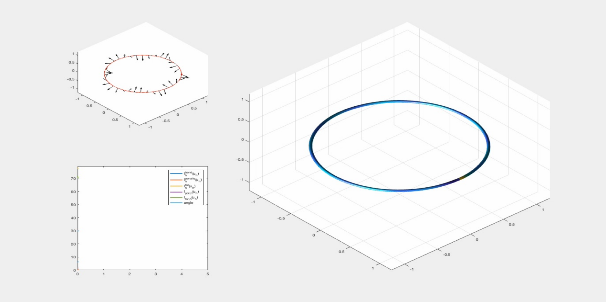
with pointwise frame condition $[u', b, d] \in SO(3)$ and rigidities $c_b = \frac{1}{2\pi} \frac{\mu(3\lambda+2\mu)}{\lambda+\mu}$ and $c_t = \frac{\mu}{2\pi}$.

H^1-coercivity in b implicit via

$$|b'|^2 = (b' \cdot u')^2 + (b' \cdot b)^2 + (b' \cdot d)^2 = (b \cdot u'')^2 + 0 + (b' \cdot d)^2$$

- not available for discretization; note $c_b \geq 2c_t$ and modify E

Gradient flow for conforming finite element discretization from flat but twisted circle with selfavoidance [B. & Reiter '21]



External Link

Material:
$c_b = 2$, $c_t = 1$

BCs:
Periodic/Dirichlet

Selfavoidance:
$\varrho = 10^{-1}$

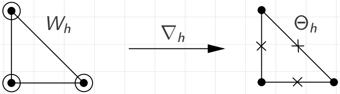
Discretization:
$h = 1/200$,
$\tau = h$, $\varepsilon = h$

- moderate drop of total twist angle
- preservation of topology and length
- occurrence of *Michell's instability*

Numerical approximation

Idea: 2d variant of splines avoiding H^2 conformity

Construction: H^1 conforming spaces W_h (cubic) and Θ_h (quadratic)



Discrete gradient: ∇_h for $w_h \in W_h$ defined as $\theta_h = \nabla_h w_h \in \Theta_h$ via

$$\theta_h(z) = \nabla w_h(z), \qquad \theta_h(z_E) \cdot n_E = \frac{1}{2}\big(\nabla w_h(z_E^1) + \nabla w_h(z_E^2)\big) \cdot n_E$$

$$\theta_h(z_E) \cdot t_E = \nabla w_h(z_E) \cdot t_E$$

for vertices $z \in \mathcal{N}_h$ and side midpoints $z_E = \big(z_E^1 + z_E^2\big)/2$

Proposition [Braess '05]: Operator $\nabla_h : W_h \to \Theta_h$ satisfies for $\ell = 0, 1$,

$$\|D^{\ell+1} w_h\|_{L^p(T)} \sim \|D^\ell \nabla_h w_h\|_{L^p(T)}, \quad \|\nabla_h w_h - \nabla w_h\|_{L^p(T)} \le ch\|D^2 w_h\|_{L^p(T)},$$

$|w_h|_{H^2_h} = \|\nabla \nabla_h w_h\|$ is semi-norm, and ∇_h interpolates $\nabla H^3(\Omega)$.

DKT discretization: For triangulation $\mathcal{T}_h$ with nodes $\mathcal{N}_h$

$$\text{Minimize} \quad I_h[y_h] = \frac{\alpha}{2}\int_\omega |\nabla\nabla_h y_h|^2 \,\mathrm{d}x - \int_\omega f_h \cdot y_h \,\mathrm{d}x$$

$$\text{subject to} \quad y_h(z) = y_D(z),\ \nabla y_h(z) = \phi_D(z) \qquad \text{f.a. } z \in \mathcal{N}_h \cap \gamma_D$$

$$\big[\nabla y_h(z)\big]^{\mathsf{T}} \nabla y_h(z) = \mathbb{I}_{2\times 2} \qquad \text{f.a. } z \in \mathcal{N}_h$$

- coercivity yields existence
- cubics: $\big(y_h(z)\big)_{z\in\mathcal{N}}$ and $\big(\nabla y_h(z)\big)_{z\in\mathcal{N}}$ are independent dof's !

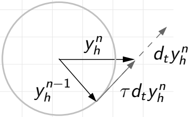
Proposition [B. '13]. Discrete (quasi-) minimizers weakly accumulate at energy minimizing H^2 isometries. Convergence is strong in H^1.

- lower bound (stability) by weak lower semicontinuity
- recovery (consistency) via interpolation of smooth approximating isometry
- only need $P2$ stiffness matrix of $-\Delta$

Gradient descent: Given $(\cdot,\cdot)_*$ compute correction $d_t y_h^n \in \mathcal{F}_h[y_h^{n-1}]$ via

$$\left(d_t y_h^n, w_h\right)_\star + \alpha\left(D_h^2 y_h^n, D_h^2 w_h\right) = \left(f_h, w_h\right)$$

for all $w_h \in \mathcal{F}_h[y_h^{n-1}]$, where



$$\mathcal{F}_h[\widehat{y}_h] = \left\{w_h \in W_h : [\nabla w_h]^\mathsf{T}\nabla\widehat{y}_h + [\nabla\widehat{y}_h]^\mathsf{T}\nabla w_h = 0 \text{ in } \mathcal{N}_h\right\}$$

and $d_t a^n = (a^n - a^{n-1})/\tau$, $D_h^2 = \nabla\nabla_h$

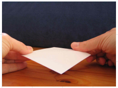
Proposition [B. '13]. If $\left[\nabla y_h^0\right]^\mathsf{T}\nabla y_h^0 = \mathbb{I}_{2\times 2}$ in $\mathcal{N}_h$ and $\|D_h^2 w_h\| \le c_\star\|w_h\|_\star$

$$\text{(i)} \quad I_h[y_h^n] + \frac{\tau}{2}\|d_t y_h^n\|_\star^2 \le I_h[y_h^{n-1}],$$

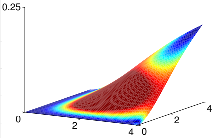
$$\text{(ii)} \quad \|[\nabla y_h^n]^\mathsf{T}\nabla y_h^n - \mathbb{I}_{2\times 2}\|_{L^1} \le c_\star^2 \tau I_h[y_h^0].$$

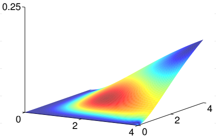
- *unconditional* stability and well-posedness, choose $w_h = d_\tau y_h^n$
- no projection – progressive violation of isometry constraint

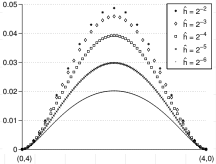
$$|G_h^n|^2 = |G_h^{n-1}|^2 + \tau^2|d_t G_h^n|^2 = \cdots = 1 + \tau^2\sum_{\ell=1}^{n}|d_t G_h^\ell|^2$$



$\omega = (0,4)\times(0,4)$, $\gamma_D = \{0\}\times[0,4]\cup[0,4]\times\{0\}$,
$y_D = (\mathrm{id},0)^{\mathsf T}$ and $\phi_D(x) = (0,0,1)^{\mathsf T}$ on Γ_D,
$f = 2.5_{-2}\cdot(0,0,1)^{\mathsf T}$, $\alpha = 1$







Discrete Gaussian curvature (displayed) and isometry errors:

$K_h = \det\left[(\nabla\nu_h)^{\mathsf T}\nabla\mathcal{I}_h y_h\right]$

$\delta I_h = (\nabla\mathcal{I}_h y_h)^{\mathsf T}\nabla\mathcal{I}_h y_h - \mathbb{I}_{2\times2}$

$\tau = h$

$\widehat{h}$	N_{iter}	$E_h(y_h)$	$\lVert\delta I_h\rVert_{L^1}$	$\lVert K_h\rVert_{L^1}$
2^{-3}	40	-9.821_{-3}	7.124_{-3}	3.043_{-3}
2^{-4}	71	-9.041_{-3}	5.143_{-3}	2.308_{-3}
2^{-5}	130	-7.666_{-3}	3.032_{-3}	1.469_{-3}
2^{-6}	272	-6.024_{-3}	1.511_{-3}	8.656_{-4}

- improvement via dG methods [Bonito, Nochetto & Ntogkas '20+]

Nonlinear bending: [Deckelnick, Dziuk & Elliott '05, Barrett, Garcke & Nürnberg '07, '12, Pozzi & Stinner '17, Walker '17, Hornung, Rumpf & Simon '19, Kovacs, Li & Lubich '20, ...]

Model extensions

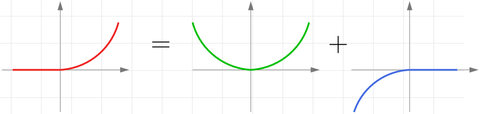
Extension I: obstacles

Approach: Include rigid obstacle $y_3(x) \leq 0$ via penalty term

$$I_{\mathrm{obs}}^{\varepsilon}[y] = \frac{1}{2}\int_\omega |D^2 y|^2 \,\mathrm{d}x + \frac{1}{2\varepsilon}\int_\omega (y_3)_+^2 \,\mathrm{d}x$$

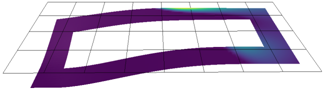
Quadratic-concave splitting: Use

$$(s)_+^2 = s^2 - (s)_-^2$$

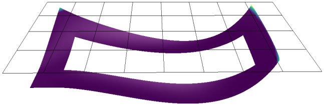


- unconditionally stable implicit-explicit iteration with linear problems

Experiments: Characterization of contact zones for single and bilayers



External Link



External Link

- nontrivial dependence of contact zone on forcing strength
- pointwise penetration control via H^2 and $W^{1,\infty}$ bounds [B. & Palus '20+]

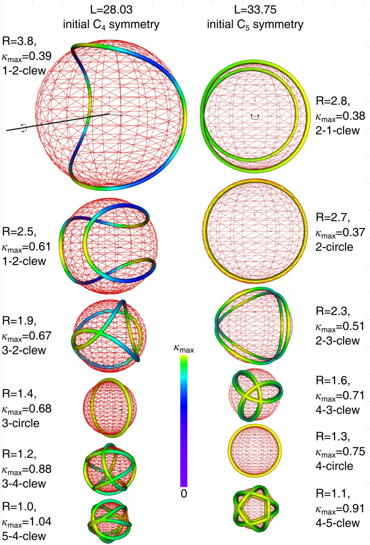
Goal: Characterize energy minimizing configurations of elastic rods of length L inside a sphere of radius R?

Obtained rods described as [B. & Weyer '21+]:

- *μ-circles*, i.e., μ times covered circles
- *μ-ν-clews*, i.e., μ-fold winding about discrete rotation axis and 2ν-fold periodicity of curvature

All rods entirely belong to sphere

Related: [Gerlach & von der Mosel '11, Dondl, Mugnai & Röger '11]



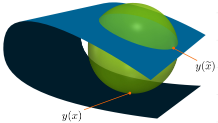
Computing injective deformations [B., Meyer & Palus '20+]

Tangent-point potential: [Gonzalez & Maddocks '99] for strength $q > 0$

$$\mathrm{TP}[y] = \frac{2^{-q}}{q} \int_\omega \int_\omega \frac{1}{r^q\big(y(x), y(\widetilde{x})\big)} \,\mathrm{d}x\,\mathrm{d}\widetilde{x}$$

with unique radius r as radius of sphere $S_r(m)$ with

- touching (tangent) in $y(x)$
- intersecting (point) in $y(\widetilde{x})$



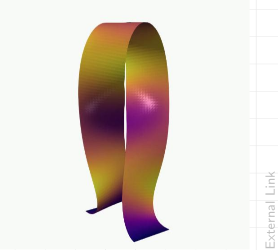
Formula:

$$r(y(x), y(\widetilde{x})) = \frac{|y(\widetilde{x}) - y(x)|^2}{2|\nu(x) \cdot (y(\widetilde{x}) - y(x))|}$$

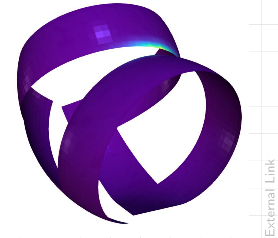
Analysis:

- self-avoidance for $q > 4$ [Strzelecki & von der Mosel '11]
- good integrability and differentiability properties [Blatt '13, Reiter '20+]
- fully explicit treatment in discrete gradient flow (no stability analysis)

Compressed strip:



Bilayer O-shaped plate:



Twisted trefoil ribbon:

Energy:

$$I[y] = I_{\mathrm{bend}}[y] + \varrho \mathrm{TP}[y]$$

Interpretation: Charged plates

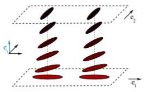
Limitations: Choice of parameters

Complexity: Parallelized assembly

CPU times: $\mathcal{O}(1d)$

Ongoing work [B., Griehl, Neukamm, Palus '20++] within DFG research unit Dresden

Setting:
- thin plate made of liquid crystal elastomer
- externally control configuration via light
- splay or twist in vertical direction

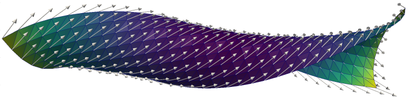


[Agostiniani & DeSimone '17]

Model: [Agostiniani & DeSimone '17] for fixed $n(x) : \omega \times (-\delta/2, \delta/2) \to \mathbb{R}^3$

$$I_{\rm lce}[y] = \frac{1}{2} \int_\omega |II - A|^2 \, \mathrm{d}x, \quad A = \gamma \begin{cases} \mathrm{diag}(-1, 1), & \text{twist} \\ \mathrm{diag}(-1, 0), & \text{splay} \end{cases}$$

Experiment: Fixed $\pi/2$-twist director (vertical), constant (horizontal)



External Link

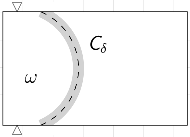
Related: Nematic elastomer sheet actuation [Plucinsky, Lemm & Bhattacharya '18]

Application: Light-fueled locomotion via optical reconfiguration [Jiang et al. '19]

Extension IV: curved folding

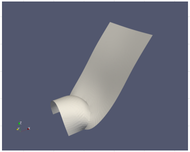
Ongoing work [B., Bonito & Hornung '21+]

Setting: Material softer/thinner along arc $C \subset \overline{\omega}$



Model reduction: $\Omega = \omega \times (-\delta/2, \delta/2)$

- narrow region C_δ, soft material $\mathbb{C}_\delta$
- ∇y discontinuous along C

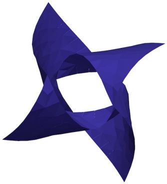


For isometry $y \in H^2(\omega \setminus C; \mathbb{R}^3) \cap W^{1,\infty}(\omega; \mathbb{R}^3)$

$$I_{\mathrm{fold}}[y] = \frac{1}{2} \int_{\omega \setminus C} |D^2 y|^2 \,\mathrm{d}x - \int_\omega f \cdot y \,\mathrm{d}x$$

Numerical scheme:

- isoparametric dG [Bonito, Nochetto & Ntogkas '20+] resolving C
- omit penalty terms along edges on C related to C^1 continuity



Related: Uniqueness [Duncan & Duncan '82], shape programming [Mahadevan '19]

Föppl-von Kármán model [Friesecke, James & Müller '06]

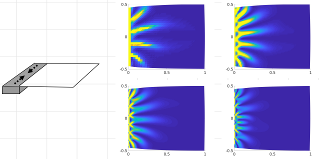
$$E_{FP}[u,w] = \frac{\gamma^2}{2}\int_\omega |D^2 w|^2 \,\mathrm{d}x + \frac{1}{2}\int_\omega |\varepsilon(u) + \nabla w \otimes \nabla w|^2 \,\mathrm{d}x$$

Numerical scheme [B. '17]:

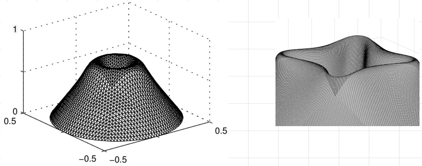
- scalar Kirchhoff elements for w, $P1$ for u
- discrete gradient flow with decoupling

Analysis: Break of symmetry [Conti, Olbermann & Tobasco '15]

Compression on one side:



Cone indentation :



Obervation: Scales in experiments highly dependent on mesh-size

Shells: [Rumpf et al. '21+]

Summary

Summary

- Wide range of applications of nonlinear bending
- Rigorously derived models in various settings
- Reliablity of discretizations via Γ convergence
- Gradient descent with linearized isometry constraint

- Ongoing and future work:
  - Stability for selfavoidance
  - Modeling dynamics
  - Constructing admissible starting values

- More information

  http://aam.uni-freiburg.de/bartels

Thank you !